

HANDBOOK OF

Aqueous Solubility Data

SECOND EDITION

**Samuel H. Yalkowsky
Yan He
Parijat Jain**



CRC Press
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CRC Press
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Boca Raton London New York

CRC Press is an imprint of the
Taylor & Francis Group, an **informa** business

CRC Press
Taylor & Francis Group
6000 Broken Sound Parkway NW, Suite 300
Boca Raton, FL 33487-2742

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CRC Press is an imprint of Taylor & Francis Group, an Informa business

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Printed in the United States of America on acid-free paper
10 9 8 7 6 5 4 3 2 1

International Standard Book Number-13: 978-1-4398-0246-5 (Ebook-PDF)

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Authors

Dr. Samuel Yalkowsky is professor of pharmaceutical sciences at the University of Arizona. He is currently involved in basic research on the relationships between chemical structure and physical phenomena such as solubility, partitioning, and melting. He has also made progress in the development of the state of the art algorithm for the estimation of the melting points, aqueous solubility and other physicochemical properties of organic compounds.

Dr. Yalkowsky is also involved in the alteration of solubility by physical means. This includes the development of formulations for insoluble drugs and the improved dissolution of environmentally important solutes from the soil. The formulation work was extended to include the development of novel dosage forms and the pharmaceutical evaluation of parenteral formulations. This has led to the development of novel methods for screening for hemolysis and for phlebitis.

Dr. Yan He earned her BS in biology from Wuhan University in 1992, her MS and PhD degrees in pharmaceutical sciences from the University of Arizona in 1999 and 2005. She is a senior research investigator in the Pharmaceuticals Sciences Department at Sanofi-Aventis. Her research interests include performing “drugability” assessment, providing formulation for preclinical studies, and preparing preformulation package for preclinical drug candidates. She also conducted basic research on the relationships between chemical structure and physical properties of organic compounds.

Dr. Parijat Jain received his PhD from the University of Arizona in 2008. Currently, he is a formulation scientist in the Pharmaceutical Development Unit at Novartis Pharmaceutical Corporation, East Hanover, NJ.

Acknowledgments

The authors would like to thank the following persons:

Mr. Jingsong Zhang for providing all the information technology support and for extracting and transforming the data to produce the final presentation for the book.

Dr. Julianne M. Braun for her assistance on the alphabetization of chemical names.

Dr. Wei-Youh Kuu and Dr. Rose-Marie Dannenfelser for the compilation of the data and the early development of this database.

Mrs. Piya Jain for assistance in the compilation of the data.

Introduction

The *Handbook of Aqueous Solubility Data* is an extensive compilation of published data for the solubility of a very wide variety of organic nonelectrolytes and unionized weak electrolytes in water. It includes data for pharmaceuticals, pollutants, nutrients, herbicides, pesticides, agricultural, industrial, and energy-related compounds. This handbook contains over sixteen thousand solubility records for more than four thousand compounds. These data were extracted from about eighteen hundred scientific references, contained in the AQUASOL dATAbASE.

Each compound is identified by a sequential number with molecular formula, compound name, synonyms, molecular weight, Chemical Abstracts Service Registry Number, melting point, and boiling point if available. For user convenience, all solubility data are converted to moles per liter and grams per liter. Also, reported numerical temperature values are converted to centigrade. The following symbols are included in the temperature field when non-numerical temperature descriptors are reported:

amb	ambient temperature
c	cold water
h	hot water
rt	room temperature
ns	temperature not stated

Each record has a five-point evaluation for the reporting of the data and a reference code for the citation. Comments are included when necessary. The following alternatives are used in the comments field:

EFG	estimated from graph
LCST	lower critical solution temperature
UCST	upper critical solution temperature

SOLUBILITY DATA

The compounds are sorted by their molecular formula using the Hill system (number of carbons, number of hydrogens, and then alphabetical by element), and then by name. Each compound can contain up to 5 synonyms. This is followed by the Chemical Abstracts Service Registry Number (RN), melting point (MP) in Celsius, molecular weight (MW), and boiling point (BP) in Celsius. Multiple values are presented whenever available. These are sorted by temperature and then by reference source.

CITATIONS

The reference citation is given as a four-character code, in which the first character is alphabetic (referring to the first author's last name) and the next three are numeric. The complete reference citation is provided in the Reference section.

EVALUATION

As listed in the Table of the Explanation of Evaluation Scores, a five-point evaluation is provided for the quality of the reporting of temperature (T), purity of solute (P), equilibration time/agitation (E), analysis (A), and accuracy and/or precision (A).

Explanation of Evaluation Scores

		Score		
Parameter		0	1	2
T	Temperature	Not given, ambient, or room temp	Given with no range	Given with range
P	Purity of solute	Not stated or as received	Stated with no range or as received	Stated with range or altered with range or calculated
E	Equilibration time/agitation	Not stated	Stated briefly	Described in detail
A	Analysis	Not stated	Stated briefly or stated in other paper	Described in detail
A	Accuracy and/or precision	1 significant figure or range > 20%	2 significant figures or range 5–20%	3 significant figures or range 1–5%

INDICES

Entries in the indices are referenced to the sequential number, not to page numbers. The formulas in Index 3 are sorted by the Hill system.

Separate indices are provided for:

Index 1: Molecular Formula

Index 2: Names and Synonyms

Index 3: Chemical Abstracts Service Registry Number (RN)

Solubility Data

1. CHBrCl₂

Bromodichloromethane

Dichlorobromomethane

BDCM

RN: 75-27-4 **MP (°C):** -55
MW: 163.83 **BP (°C):** 87

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.851E-02	3.032E+00	30	M300	1 1 2 2 2	
1.812E-02	2.968E+00	30	M311	1 1 2 2 2	

2. CHBr₂Cl

Chlorodibromomethane

Dibromochloromethane

CDBM

RN: 124-48-1 **MP (°C):** -22
MW: 208.29 **BP (°C):** 119.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.041E-03	1.050E+00	30	M300	1 1 2 2 2	
1.205E-02	2.509E+00	30	M311	1 1 2 2 2	

3. CHBr₃

Bromoform

Tribromomethane

Methyl tribromide

RN: 75-25-2 **MP (°C):** 7.5
MW: 252.75 **BP (°C):** 149

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.187E-02	3.001E+00	15	G029	1 0 2 2 2	
3.957E-03	1.000E+00	20	F300	1 0 0 0 0	
<7.91E-04	<2.00E-01	25	B019	1 0 1 2 0	sic
1.262E-02	3.190E+00	30	F300	1 0 0 0 2	
1.258E-02	3.180E+00	30	G029	1 0 2 2 2	
1.555E-02	3.931E+00	30	M311	1 1 2 2 2	
1.256E-02	3.174E+00	30	V009	1 0 0 0 2	
1.227E-02	3.100E+00	ns	O006	0 0 0 0 2	

4. CHClF₂

Chlorodifluoromethane

Freon 22

Halocarbon 22

RN: 75-45-6**MP (°C):** -146**MW:** 86.47**BP (°C):** -40.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.018E-01	2.610E+01	21	M065	1 0 2 1 2	

5. CHCl₃

Chloroform

Trichloromethane

Methyl trichloride

Formyl trichloride

RN: 67-66-3**MP (°C):** -63**MW:** 119.38**BP (°C):** 61

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.896E-02	1.062E+01	0	H101	2 0 0 0 2	
7.077E-02	8.448E+00	15	G029	1 0 2 2 2	
7.134E-02	8.517E+00	15	J036	0 0 0 0 0	
6.648E-02	7.937E+00	20	E019	1 0 1 1 0	
6.785E-02	8.100E+00	20	F300	1 0 0 0 1	
6.886E-02	8.220E+00	20	H101	2 0 0 0 2	
6.869E-02	8.200E+00	20	M133	1 0 0 0 2	
6.827E-02	8.150E+00	20	M368	1 0 0 0 1	
6.648E-02	7.937E+00	20	N034	1 0 0 0 0	
6.869E-02	8.200E+00	20	P046	1 0 0 0 0	
6.750E-02	8.058E+00	20	P073	1 0 0 1 2	
3.504E-02	4.182E+00	22	H072	1 0 1 1 2	
7.472E-02	8.920E+00	25	B019	1 0 1 2 0	
6.050E-02	7.222E+00	25	B173	2 0 2 2 2	
6.660E-02	7.950E+00	25	F071	1 1 2 1 2	
6.648E-02	7.937E+00	25	G056	1 0 0 0 2	
6.813E-02	8.133E+00	25	L319	1 0 2 1 2	
6.618E-02	7.900E+00	25	M037	1 1 0 0 1	
6.648E-02	7.937E+00	25	O026	1 2 0 1 0	
7.472E-02	8.920E+00	25	R321	1 2 1 1 1	
6.236E-02	7.444E+00	25.0	C055	1 2 1 0 1	
6.409E-02	7.651E+00	30	G029	1 0 2 2 2	
6.500E-02	7.760E+00	30	H101	2 0 0 0 2	
2.114E-02	2.524E+00	30	M311	1 1 2 2 2	
6.411E-02	7.653E+00	30	V009	1 0 0 0 2	
6.648E-02	7.937E+00	56.1	C055	2 2 1 0 0	
6.236E-02	7.444E+00	60	R321	1 2 1 1 1	
6.660E-02	7.950E+00	ns	H123	0 0 0 0 0	

(continued)

5. CHCl₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.168E-02	4.975E+00	ns	I306	0 0 0 0 0	
6.660E-02	7.950E+00	ns	M344	0 0 0 0 2	
6.830E-02	8.153E+00	ns	R028	0 0 0 0 0	

6. CHI₃

Iodoform

Triiodomethane

RN: 75-47-8 **MP (°C):** 121.5
MW: 393.73 **BP (°C):** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	1.181E-01	25	V009	1 0 0 0 0	
2.540E-04	9.999E-02	rt	D021	0 0 1 1 0	

7. CH₂BrCl

Bromochloromethane

Bromo-chloro-methane

Chlorobromomethane

CBM

RN: 74-97-5 **MP (°C):** -86.5
MW: 129.39 **BP (°C):** 68.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-01	1.669E+01	25	M342	1 0 1 1 2	
1.142E-01	1.478E+01	ns	O006	0 0 0 0 1	

8. CH₂Br₂

Methylene bromide

Dibrom-methan

RN: 74-95-3 **MP (°C):** -52.7
MW: 173.85 **BP (°C):** 97

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.747E-02	1.173E+01	0	H101	2 0 0 0 2	
6.652E-02	1.156E+01	15	G029	1 0 2 2 2	
6.604E-02	1.148E+01	20	H101	2 0 0 0 2	
6.259E-02	1.088E+01	25	O006	1 0 0 0 1	
6.782E-02	1.179E+01	30	G029	1 0 2 2 2	

(continued)

8. CH₂Br₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.765E-02	1.176E+01	30	H101	2 0 0 0 2	
6.779E-02	1.179E+01	30	V009	1 0 0 0 2	
6.558E-02	1.140E+01	ns	F300	0 0 0 0 2	

9. CH₂Cl₂

Methylene chloride

Dichlor-methan

Dichloromethane

Methylene dichloride

Methane dichloride

RN: 75-09-2

MP (°C): -95.1

MW: 84.93

BP (°C): 39.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.782E-01	2.363E+01	0	H101	2 0 0 0 2	
2.309E-01	1.961E+01	20	C057	0 0 0 0 0	
2.355E-01	2.000E+01	20	F300	1 0 0 0 0	
2.355E-01	2.000E+01	20	H101	2 0 0 0 2	
2.263E-01	1.922E+01	20	N034	1 0 0 0 2	
1.887E-01	1.603E+01	20	N038	1 0 0 1 2	
2.309E-01	1.961E+01	25	A094	1 0 0 0 1	
1.534E-01	1.303E+01	25	G056	1 0 0 0 2	
1.554E-01	1.320E+01	25	M037	1 1 0 0 2	
1.554E-01	1.320E+01	25	M133	1 0 0 0 2	
1.554E-01	1.320E+01	25	P046	1 0 0 0 0	
2.275E-01	1.932E+01	30	V009	1 0 0 0 2	
2.284E-01	1.940E+01	ns	H123	0 0 0 0 0	

10. CH₂I₂

Methylene iodide

Diiod-methan

RN: 75-11-6

MP (°C): 6.0

MW: 267.84

BP (°C): 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.110E-03	8.330E-01	25	A032	1 2 1 1 2	
4.624E-03	1.238E+00	30	G029	1 0 2 2 2	
4.594E-03	1.231E+00	30	V009	1 0 0 0 1	

11. CH₂N₂

Cyanamide
Cyanamid

RN: 420-04-2 **MP (°C):**
MW: 42.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E+01	4.444E+02	ns	N013	0 0 0 0 1	

12. CH₃Br

Methyl bromide
Bromomethane
Celfume

RN: 74-83-9 **MP (°C):** -94
MW: 94.94 **BP (°C):** 3.56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.748E-01	2.609E+01	10	H081	1 0 2 0 2	
1.893E-01	1.797E+01	17	H081	1 0 2 0 2	
1.893E-01	1.797E+01	17	M061	1 0 0 0 2	
1.933E-01	1.835E+01	19.9	G061	1 2 1 1 2	774.3mm Hg @ 25 °C
1.685E-01	1.600E+01	20	G080	1 0 0 0 1	
1.659E-01	1.575E+01	20	P081	1 0 0 0 1	
1.394E-01	1.323E+01	25	H081	1 0 2 0 2	
1.411E-01	1.340E+01	25	M161	1 0 0 0 2	
1.196E-01	1.136E+01	32	H081	1 0 2 0 2	
9.479E-03	9.000E-01	ns	N013	0 0 0 0 1	

13. CH₃BrO₆S₂

Bromomethionic acid
Methanedisulfonic acid, bromo-

RN: 187610-86-2 **MP (°C):**
MW: 255.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.039E+00	7.752E+02	25	B077	1 2 0 0 2	

14. CH₃Cl

Methyl chloride

Chloromethane

RN: 74-87-3**MP (°C):** -97.0**MW:** 50.49**BP (°C):** -23.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E+01	7.727E+02	0	M061	1 0 0 0 1	<i>sic</i>
1.436E-01	7.250E+00	20	M133	1 0 0 0 2	
9.069E-02	4.579E+00	20	N034	1 0 0 0 1	
1.436E-01	7.250E+00	20	P046	1 0 0 0 0	
1.059E-01	5.347E+00	24.9	G061	1 2 1 1 2	756.1mm Hg @ 25 °C
1.455E-01	7.346E+00	30	G056	1 0 0 0 2	
1.466E-01	7.400E+00	30	M037	1 1 0 0 1	

15. CH₃ClO₆S₂

Chloromethionic acid

Acide chlorométhionique

RN: 74692-14-1 **MP (°C):****MW:** 210.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.540E+01	3.243E+03	25	B075	1 2 0 0 2	

16. CH₃F

Fluoromethane

Methylfluoride

RN: 593-53-3 **MP (°C):** -141.8**MW:** 34.03 **BP (°C):** -78.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~7.05E-02	~2.40E+00	15	F300	1 0 0 0 0	
5.250E-02	1.787E+00	29.9	G061	1 2 1 1 2	766.8mm Hg @25 °C

17. CH₃I

Iodomethane
Methyl-iodide
Halon 10001
Methyl iodine
Methyliodide

RN: 74-88-4 **MP (°C):** -64
MW: 141.94 **BP (°C):** 42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E-01	1.565E+01	0	H101	2 0 0 0 2	
9.997E-02	1.419E+01	20	H101	2 0 0 0 2	
9.727E-02	1.381E+01	20	H127	1 0 0 0 1	
9.727E-02	1.381E+01	20	I316	0 0 0 0 0	
9.600E-02	1.363E+01	20	M171	1 0 0 0 2	
9.590E-02	1.361E+01	22	F001	1 0 1 2 2	
9.511E-02	1.350E+01	22	F300	1 0 0 0 2	
9.590E-02	1.361E+01	22	S006	1 0 0 0 2	
1.007E-01	1.429E+01	30	H101	2 0 0 0 2	
9.957E-02	1.413E+01	30	V009	1 0 0 0 2	
8.725E-03	1.238E+00	ns	O006	0 0 0 0 1	

18. CH₃NO

Formaldehyde oxime
Formaldehyd-oxim

RN: 75-17-2 **MP (°C):**
MW: 45.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.774E+00	1.700E+02	20	F300	1 0 0 0 1	

19. CH₃NO₂

Nitromethane
Nitrocarbol
NM

RN: 75-52-5 **MP (°C):** -29
MW: 61.04 **BP (°C):** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.421E+00	8.676E+01	20	C121	0 0 0 0 1	unit assumed, <i>sic</i>
1.627E+00	9.934E+01	25	F049	2 0 2 0 0	
1.802E+00	1.100E+02	25	M136	2 0 0 0 2	
1.802E+00	1.100E+02	25	M139	2 0 0 0 2	
3.039E-01	1.855E+01	ns	D348	0 0 0 0 0	

20. CH₃N₅

5-Aminotetrazole

5-Amino-tetrazol

RN: 4418-61-5**MP (°C):** 204**MW:** 85.07**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.411E-01	1.200E+01	18	F300	1 0 0 0 1	

21. CH₄

Methane

Methan

RN: 74-82-8**MP (°C):** -183**MW:** 16.04**BP (°C):** -161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.468E-03	3.960E-02	0	F300	1 0 0 0 2	
2.210E-03	3.545E-02	4.99	C115	2 0 2 2 2	
1.926E-03	3.090E-02	9.99	C115	2 0 2 2 2	
1.633E-03	2.620E-02	14.99	C115	2 0 2 2 2	
1.567E-03	2.513E-02	19.8	G058	1 0 0 0 2	
1.511E-03	2.424E-02	19.99	C115	2 0 2 2 2	
1.446E-03	2.320E-02	20	F300	1 0 0 0 2	
1.381E-03	2.215E-02	24.99	C115	2 0 2 2 2	
1.521E-03	2.440E-02	25	M001	2 1 2 2 2	
1.521E-03	2.440E-02	25	M002	2 2 1 2 2	
1.502E-03	2.410E-02	25	M040	1 0 0 1 2	
1.550E-03	2.487E-02	25	M102	1 2 2 1 2	
1.266E-03	2.030E-02	29.99	C115	2 0 2 2 2	
1.189E-03	1.907E-02	34.99	C115	2 0 2 2 2	
1.079E-03	1.732E-02	39.99	C115	2 0 2 2 2	
1.056E-03	1.693E-02	40	S212	2 1 2 2 2	
1.055E-03	1.693E-02	44.99	C115	2 0 2 2 2	
8.477E-04	1.360E-02	50	F300	1 0 0 0 2	
9.000E-04	1.444E-02	60	S212	2 1 2 2 2	
8.000E-04	1.283E-02	80	S212	2 1 2 2 2	
1.434E-03	2.300E-02	ns	M091	0 1 0 0 2	
1.378E-03	2.210E-02	ns	S212	2 1 2 2 2	

22. CH₄N₂O

Urea

Harnstoff

Uree

RN: 57-13-6**MP (°C):** 132.7**MW:** 60.06**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.680E+00	4.012E+02	0	F300	1 0 0 0 2	
4.757E+00	2.857E+02	0	J021	1 0 0 0 2	
6.680E+00	4.012E+02	0	M043	1 0 0 0 1	
6.680E+00	4.012E+02	0	P023	1 2 1 1 2	
7.297E+00	4.382E+02	5	D041	1 0 0 0 1	
5.088E+00	3.056E+02	7	J021	1 0 0 0 2	
5.246E+00	3.151E+02	10	D020	1 2 1 1 2	
5.246E+00	3.151E+02	10	D060	2 2 1 1 2	
7.651E+00	4.595E+02	10	M043	1 0 0 0 1	
7.602E+00	4.565E+02	10	P023	1 2 1 1 2	
5.550E+00	3.333E+02	17	J021	1 0 0 0 2	
7.382E+00	4.433E+02	18.72	S131	2 2 1 1 2	recrystallized
5.536E+00	3.324E+02	20	C052	1 2 1 1 2	
5.617E+00	3.373E+02	20	J021	1 0 0 0 2	
8.529E+00	5.122E+02	20	M043	1 0 0 0 2	
8.517E+00	5.115E+02	20	P023	1 2 1 1 2	
7.594E+00	4.561E+02	21.59	S131	2 2 1 1 2	recrystallized
7.738E+00	4.647E+02	23.85	S131	2 2 1 1 2	recrystallized
5.874E+00	3.528E+02	25	D020	1 2 1 1 2	
9.058E+00	5.440E+02	25	D041	1 0 0 0 2	
5.874E+00	3.528E+02	25	D060	2 2 1 1 2	
8.326E+00	5.000E+02	25	M136	2 0 0 0 2	
7.910E+00	4.750E+02	26.83	S131	2 2 1 1 2	recrystallized
7.966E+00	4.784E+02	27.31	S131	2 2 1 1 2	recrystallized
9.566E+00	5.745E+02	30	M043	1 0 0 0 2	
9.596E+00	5.763E+02	30	P023	1 2 1 1 2	
8.171E+00	4.907E+02	30.38	S131	2 2 1 1 2	recrystallized
6.244E+00	3.750E+02	35	J021	1 0 0 0 2	
1.712E+01	1.028E+03	35	S200	1 0 0 0 2	loc. cit.
8.469E+00	5.086E+02	35.15	S131	2 2 1 1 2	recrystallized
8.465E+00	5.083E+02	35.42	S131	2 2 1 1 2	recrystallized
8.575E+00	5.150E+02	37.36	S131	2 2 1 1 2	recrystallized
1.038E+01	6.232E+02	39.7	P023	1 2 1 1 2	
6.392E+00	3.839E+02	40	D020	1 2 1 1 2	
6.392E+00	3.839E+02	40	D060	2 2 1 1 2	
1.037E+01	6.226E+02	40	M043	1 0 0 0 2	
1.837E+01	1.103E+03	40	S200	1 0 0 0 2	loc. cit.
8.822E+00	5.298E+02	41.11	S131	2 2 1 1 2	recrystallized
8.982E+00	5.394E+02	43.85	S131	2 2 1 1 2	recrystallized
8.967E+00	5.386E+02	43.94	S131	2 2 1 1 2	recrystallized
1.961E+01	1.178E+03	45	S200	1 0 0 0 2	loc. cit.
9.107E+00	5.469E+02	46.56	S131	2 2 1 1 2	recrystallized
1.119E+01	6.721E+02	50	P023	1 2 1 1 2	

(continued)

22. CH₄N₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E+01	1.267E+03	50	S200	1 0 0 0 2	loc. cit.
1.122E+01	6.736E+02	50.6	P023	1 2 1 1 2	
9.560E+00	5.742E+02	54.77	S131	2 2 1 1 2	recrystallized
9.584E+00	5.756E+02	54.97	S131	2 2 1 1 2	recrystallized
2.283E+01	1.371E+03	55	S200	1 0 0 0 2	loc. cit.
9.649E+00	5.795E+02	55.88	S131	2 2 1 1 2	recrystallized
9.681E+00	5.814E+02	57.02	S131	2 2 1 1 2	recrystallized
9.806E+00	5.889E+02	59.13	S131	2 2 1 1 2	recrystallized
6.936E+00	4.166E+02	60	J021	1 0 0 0 2	
9.847E+00	5.914E+02	60	K013	1 0 1 1 2	
1.189E+01	7.143E+02	60	M043	1 0 0 0 2	
2.422E+01	1.455E+03	60	S200	1 0 0 0 2	loc. cit.
1.184E+01	7.110E+02	60.0	P023	1 2 1 1 2	
9.930E+00	5.963E+02	61.76	S131	2 2 1 1 2	recrystallized
1.005E+01	6.034E+02	63.79	S131	2 2 1 1 2	recrystallized
1.009E+01	6.060E+02	65	K013	1 0 1 1 2	
2.570E+01	1.543E+03	65	S200	1 0 0 0 2	loc. cit.
1.244E+01	7.468E+02	68.5	P023	1 2 1 1 2	
1.020E+01	6.127E+02	68.50	M059	1 1 2 1 2	
1.270E+01	7.629E+02	70	F300	1 0 0 0 2	
7.206E+00	4.328E+02	70	J021	1 0 0 0 2	
1.033E+01	6.206E+02	70	K013	1 0 1 1 2	
1.263E+01	7.588E+02	70	P023	1 2 1 1 2	
2.730E+01	1.640E+03	70	S200	1 0 0 0 2	loc. cit.
1.038E+01	6.231E+02	70.49	S131	2 2 1 1 2	recrystallized
1.048E+01	6.295E+02	73.11	S131	2 2 1 1 2	recrystallized
1.057E+01	6.345E+02	75	K013	1 0 1 1 2	
1.048E+01	6.296E+02	75.30	M059	1 1 2 1 2	
1.079E+01	6.480E+02	80	K013	1 0 1 1 2	
1.332E+01	8.000E+02	80	M043	1 0 0 0 2	
1.090E+01	6.546E+02	84.40	M059	1 1 2 1 2	
1.101E+01	6.610E+02	85	K013	1 0 1 1 2	
3.229E+01	1.939E+03	85	S200	1 0 0 0 2	loc. cit.
1.122E+01	6.738E+02	90	K013	1 0 1 1 2	
3.426E+01	2.058E+03	90	S200	1 0 0 0 2	loc. cit.
1.131E+01	6.791E+02	93.80	M059	1 1 2 1 2	
1.142E+01	6.858E+02	95	K013	1 0 1 1 2	
3.611E+01	2.169E+03	95	S200	1 0 0 0 2	loc. cit.
1.161E+01	6.975E+02	100	K013	1 0 1 1 2	
1.465E+01	8.795E+02	100	M043	1 0 0 0 2	
3.778E+01	2.269E+03	100	S200	1 0 0 0 2	loc. cit.
1.177E+01	7.066E+02	104.40	M059	1 1 2 1 2	
1.199E+01	7.199E+02	109.90	M059	1 1 2 1 2	
1.219E+01	7.321E+02	115.30	M059	1 1 2 1 2	
1.229E+01	7.383E+02	118.30	M059	1 1 2 1 2	
1.234E+01	7.411E+02	118.70	M059	1 1 2 1 2	
1.245E+01	7.479E+02	121.90	M059	1 1 2 1 2	
1.249E+01	7.503E+02	123.20	M059	1 1 2 1 2	
1.264E+01	7.592E+02	127.50	M059	1 1 2 1 2	

(continued)

22. CH₄N₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.269E+01	7.619E+02	128.80	M059	1 1 2 1 2	
1.281E+01	7.694E+02	132.60	M059	1 1 2 1 2	
1.665E+01	1.000E+03	ns	B338	0 0 0 0 1	
1.332E+01	8.000E+02	ns	D072	0 0 0 0 0	

23. CH₄N₂S

Thiourea

Thiouree

RN: 62-56-6 MP (°C): 176
 MW: 76.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.136E-01	4.671E+01	0	M043	1 0 0 0 1	
9.731E-01	7.407E+01	10	M043	1 0 0 0 1	
1.118E+00	8.507E+01	10	O017	1 0 1 1 2	
1.206E+00	9.180E+01	13	F300	1 0 0 0 2	
1.206E+00	9.179E+01	13	O019	1 0 0 1 2	
1.383E+00	1.053E+02	15	O017	1 0 1 1 2	
1.573E+00	1.197E+02	20	M043	1 0 0 0 2	
1.544E+00	1.175E+02	20	O017	1 0 1 1 2	
1.085E+00	8.257E+01	25	I310	0 0 0 0 0	
1.759E+00	1.339E+02	25	O017	1 0 1 1 2	
2.199E+00	1.674E+02	30	M043	1 0 0 0 2	
3.093E+00	2.355E+02	40	M043	1 0 0 0 2	
5.455E+00	4.152E+02	60	M043	1 0 0 0 1	
7.617E+00	5.798E+02	80	M043	1 0 0 0 2	
9.250E+00	7.041E+02	100	M043	1 0 0 0 2	
7.882E-01	6.000E+01	ns	D072	0 0 0 0 0	

24. CH₄N₄O₂

α-Nitroguanidine

Nitroguanidine

Nitroguanidin

RN: 556-88-7 MP (°C): 235
 MW: 104.07 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.597E-02	2.703E+00	19.5	D027	1 2 0 0 2	
1.173E-01	1.221E+01	25	D022	1 1 2 2 2	
4.228E-02	4.400E+00	25	F300	1 0 0 0 1	
4.305E-02	4.480E+00	29.87	M028	1 2 2 1 0	EFG
1.122E-01	1.167E+01	50	D027	1 2 0 0 2	
3.070E-01	3.195E+01	71.67	M028	1 2 2 1 0	EFG
5.695E-01	5.927E+01	83.98	M028	1 2 2 1 0	EFG
9.025E-01	9.392E+01	100	D027	1 2 0 0 2	
7.620E-01	7.930E+01	100	F300	1 0 0 0 2	

25. CH₄O

Methanol

Methyl alcohol

RN: 67-56-1

MP (°C): -97.8

MW: 32.04

BP (°C): 64.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.689E+01	5.411E+02	ns	L003	0 0 2 1 2	

26. CH₄O₆S₂

Methionic acid

Acide methionique

Methanedisulfonic acid

RN: 503-40-2

MP (°C): 98.0

MW: 176.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.395E+01	2.458E+03	25	B075	1 2 0 0 2	
4.035E+00	7.108E+02	25	B076	1 2 0 0 2	
4.862E+00	8.566E+02	25	F300	1 0 0 0 2	

27. CH₄O₆S₂.H₂O

Methionic acid (monohydrate)

RN: 503-40-2

MP (°C):

MW: 194.18

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.409E+00	8.562E+02	25	B076	1 2 0 0 2	

28. CH₅N

Methylamine

Aminomethane

Carbinamine

Mercurialin

RN: 74-89-5

MP (°C): -93.5

MW: 31.06

BP (°C): -6.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.906E+01	5.920E+02	4.50	F300	1 0 0 0 2	
2.963E+01	9.202E+02	12.5	D041	1 0 0 0 2	
2.147E+01	6.667E+02	12.50	M081	1 0 0 0 2	
1.916E+01	5.951E+02	20	M081	1 0 0 0 2	

(continued)

28. CH₅N (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.789E+01	5.556E+02	25	M081	1 0 0 0 2	
1.664E+01	5.169E+02	30	M081	1 0 0 0 2	
1.380E+01	4.286E+02	40	M081	1 0 0 0 1	
1.143E+01	3.548E+02	50	M081	1 0 0 0 1	
9.034E+00	2.806E+02	60	M081	1 0 0 0 1	

29. CH₅N₅O₂

Nitroaminoguanidine

Hydrazinecarboximidamide, *N*-nitro-

1-Amino-3-nitroguanidine

3-Amino-1-nitroguanidine

1-Amino-2-nitroguanidine

1-Nitro-3-aminoguanidine

RN: 18264-75-0 MP (°C): 185

MW: 119.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	1.619E+00	9.33	M047	2 2 1 1 0	EFG
2.254E-02	2.684E+00	20.96	M047	2 2 1 1 0	EFG
3.567E-02	4.248E+00	29.87	M047	2 2 1 1 0	EFG
4.384E-02	5.221E+00	34.53	M047	2 2 1 1 0	EFG
7.087E-02	8.440E+00	44.30	M047	2 2 1 1 0	EFG
9.318E-02	1.110E+01	49.42	M047	2 2 1 1 0	EFG

30. CH₅O₃As

Methanearsonic acid

MAA

Methylarsonsaeure

RN: 124-58-3 MP (°C): 132

MW: 139.97 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E+00	2.038E+02	20	B200	1 0 0 0 2	
1.563E+00	2.188E+02	25	D305	1 0 0 0 1	

31. CH₅As

Methylarsine

Methylarsin

RN: 593-52-2

MP (°C): -143

MW: 91.97

BP (°C): 2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.242E-04	8.500E-02	20	F300	1 0 0 0 1	

32. CBrClF₂

Bromochlorodifluoromethane

Halon 1211

Chlorodifluorobromomethane

Bromochlorodifluoromethine

RN: 353-59-3

MP (°C):

MW: 165.37

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.555E-05	1.580E-02	0	G055	1 2 2 2 1	

33. CBr₃F

Tribromo-fluoro-methane

Methane, tribromofluoro-

Fluorotribromomethane

RN: 353-54-8

MP (°C):

MW: 270.74

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.477E-03	3.998E-01	25	O006	1 0 0 0 1	

34. CBr₄

Carbon tetrabromide

Tetrabromomethane

RN: 558-13-4

MP (°C): 89

MW: 331.65

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.235E-04	2.399E-01	30	G029	1 0 2 2 1	
6.998E-04	2.321E-01	30	V009	1 0 0 0 0	

35. CCN

Cyanogen chloride

Chlorcyan

RN: 506-77-4

MP (°C): -6

MW: 61.47

BP (°C): 13.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.761E-01	6.000E+01	0	F300	1 0 0 0 0	

36. CCIN₃O₆

Chlorotrinitromethane

Chlor-trinitro-methan

RN: 1943-16-4

MP (°C):

MW: 185.48

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.186E-02	2.200E+00	20	F300	1 0 0 0 1	

37. CCl₂F₂

Dichlorodifluoromethane

Difluorodichloromethane

Freon 12

RN: 75-71-8

MP (°C): -158

MW: 120.91

BP (°C): -29.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.544E-02	1.867E+00	21	M065	1 0 2 1 2	
2.316E-03	2.800E-01	25	M133	1 0 0 0 2	
2.316E-03	2.800E-01	25	P046	1 0 0 0 0	
2.315E-03	2.799E-01	25	R048	0 0 0 0 0	

38. CCl₃F

Trichlorofluoromethane

Fluorotrichloromethane

Freon 11

RN: 75-69-4

MP (°C): -111

MW: 137.37

BP (°C): 23.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.401E+00	20	H041	0 0 0 0 0	
8.008E-03	1.100E+00	20	M133	1 0 0 0 2	
8.008E-03	1.100E+00	20	P046	1 0 0 0 0	
1.020E-02	1.401E+00	21	H041	0 0 0 0 0	

(continued)

38. CCl₃F (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.013E-03	1.101E+00	25	H041	0 0 0 0 0	
7.999E-03	1.099E+00	25	R048	0 0 0 0 0	
7.997E-03	1.099E+00	27	H041	0 0 0 0 0	
7.853E-03	1.079E+00	30	H041	0 0 0 0 0	
9.892E-03	1.359E+00	31	H041	0 0 0 0 0	
4.152E-03	5.703E-01	50	H041	0 0 0 0 0	
2.258E-03	3.102E-01	75	H041	0 0 0 0 0	

39. CCl₃NO₂

Chloropicrin

Chlorpikrin

RN: 76-06-2

MP (°C): -64

MW: 164.38

BP (°C): 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	2.270E+00	0	M161	1 0 0 0 2	
1.396E-02	2.295E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>
1.186E-02	1.950E+00	20	G080	1 0 0 0 1	
9.718E-03	1.597E+00	20	M061	1 0 0 0 1	
1.214E-02	1.996E+00	20	P081	1 0 0 0 0	
9.874E-03	1.623E+00	25	F300	1 0 0 0 2	
1.217E-02	2.000E+00	ns	N013	0 0 0 0 2	

40. CCl₄

Carbon tetrachloride

Tetrachloromethane

Methane tetrachloride

RN: 56-23-5

MP (°C): -23

MW: 153.82

BP (°C): 76.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.306E-03	9.700E-01	0	H101	2 0 0 0 1	
5.002E-03	7.694E-01	15	G029	1 0 2 2 1	
5.002E-03	7.694E-01	15	J036	0 0 0 0 0	
5.197E-03	7.994E-01	20	C121	1 0 0 0 0	unit assumed, <i>sic</i>
5.201E-03	8.000E-01	20	H101	2 0 0 0 1	
5.201E-03	8.000E-01	20	M040	1 0 0 1 2	
5.103E-03	7.850E-01	20	M133	1 0 0 0 2	
5.200E-03	7.999E-01	20	M312	1 0 0 0 2	
4.612E-03	7.095E-01	20	N038	1 0 0 1 2	
5.103E-03	7.850E-01	20	P046	1 0 0 0 0	

(continued)

40. CCl₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.494E-03	9.990E-01	25	B019	1 0 1 2 0	
4.920E-03	7.568E-01	25	B173	2 0 2 2 2	
5.000E-03	7.691E-01	25	G038	1 2 2 2 1	
5.000E-03	7.691E-01	25	G053	2 1 2 1 1	
5.197E-03	7.994E-01	25	G056	1 0 0 0 2	
5.197E-03	7.994E-01	25	L319	1 0 2 1 1	
5.201E-03	8.000E-01	25	M037	1 1 0 0 0	
5.197E-03	7.994E-01	25	M061	1 0 0 0 0	
1.820E-03	2.800E-01	25	M161	1 0 0 0 1	
5.006E-03	7.700E-01	25	M368	1 0 0 0 1	
1.038E-02	1.597E+00	25	N034	1 0 0 0 1	sic
5.556E-03	8.546E-01	25	S133	1 1 1 1 1	
5.262E-03	8.093E-01	30	G029	1 0 2 2 1	
5.526E-03	8.500E-01	30	H101	2 0 0 0 1	
5.296E-03	8.146E-01	30	V009	1 0 0 0 1	
5.201E-03	8.000E-01	ns	F071	0 1 2 1 2	
5.201E-03	8.000E-01	ns	H080	0 0 0 0 2	
3.249E-03	4.998E-01	ns	I306	0 0 0 0 0	
5.201E-03	8.000E-01	ns	M344	0 0 0 0 2	

41. CF₄

Carbon tetrafluoride

Tetrafluoromethane

RN: 75-73-0 MP (°C): -184
 MW: 88.00 BP (°C): -128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.319E-04	2.041E-02	19.99	C115	2 0 2 2 2	
2.083E-04	1.833E-02	24.99	C115	2 0 2 2 2	
2.111E-04	1.858E-02	25	D055	1 0 0 0 1	
1.940E-04	1.707E-02	29.99	C115	2 0 2 2 2	

42. COS

Carbonyl sulfide

Kohlenoxidsulfid

RN: 463-58-1 MP (°C): -138
 MW: 60.07 BP (°C): -50

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.259E-02	3.760E+00	0	F300	1 0 0 0 2	
2.081E-02	1.250E+00	25	F300	1 0 0 0 2	

43. CO₂

Carbon dioxide

Carbonic acid gas

Carbonic anhydride

RN: 124-38-9**MP (°C):** -57**MW:** 44.01**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.641E-02	3.803E+00	16	B109	1 0 0 0 2	unit assumed, <i>sic</i>
8.377E-02	3.687E+00	17	B109	1 0 0 0 2	unit assumed, <i>sic</i>
8.641E-02	3.803E+00	18	B109	1 0 0 0 2	unit assumed, <i>sic</i>
8.123E-02	3.575E+00	18	B109	1 0 0 0 2	unit assumed, <i>sic</i>
7.886E-02	3.471E+00	19	B109	1 0 0 0 2	unit assumed, <i>sic</i>
7.654E-02	3.369E+00	20	B109	1 0 0 0 2	unit assumed, <i>sic</i>
7.432E-02	3.271E+00	21	B109	1 0 0 0 2	unit assumed, <i>sic</i>
7.427E-02	3.269E+00	21	B109	1 0 0 0 2	unit assumed, <i>sic</i>
7.213E-02	3.174E+00	22	B109	1 0 0 0 2	unit assumed, <i>sic</i>
6.582E-02	2.897E+00	25	B109	1 0 0 0 2	unit assumed, <i>sic</i>
3.360E-02	1.479E+00	25	H124	1 0 0 1 2	
6.204E-02	2.730E+00	27	B109	1 0 0 0 2	unit assumed, <i>sic</i>
6.127E-02	2.696E+00	28	B109	1 0 0 0 2	unit assumed, <i>sic</i>
5.714E-02	2.515E+00	30	B109	1 0 0 0 2	unit assumed, <i>sic</i>

44. CS₂

Carbon disulfide

Carbon disulphide

Schwefelkohlenstoff

RN: 75-15-0**MP (°C):** -112**MW:** 76.14**BP (°C):** 46.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.679E-02	2.040E+00	0	F300	1 0 0 0 2	
3.257E-02	2.480E+00	0	H101	2 0 0 0 2	
2.883E-02	2.195E+00	20	C121	0 0 0 0 1	unit assumed, <i>sic</i>
2.351E-02	1.790E+00	20	F300	1 0 0 0 2	
2.850E-02	2.170E+00	20	G080	1 0 0 0 1	
2.844E-02	2.165E+00	20	M061	1 0 0 0 2	
3.850E-02	2.931E+00	20	N038	1 0 0 1 2	
2.889E-02	2.200E+00	22	P076	1 2 1 1 1	
3.746E-02	2.852E+00	25	L319	1 0 2 1 1	
2.036E-02	1.550E+00	30	F300	1 0 0 0 2	
2.889E-02	2.200E+00	32	M161	1 0 0 0 1	
2.627E-02	2.000E+00	ns	N013	0 0 0 0 2	

45. C₂HBrClF₃

Halothane

2-Bromo-2-chloro-1,1,1-trifluoroethane

Fluothane

RN: 151-67-7**MP (°C):** <25**MW:** 197.39**BP (°C):** 50.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-02	3.438E+00	ns	R028	0 0 0 0 0	

46. C₂HCl₃

Trichloroethylene

Trichloroethene

Trichloro-ethylene

Ethyne trichloride

Acetylene trichloride

1,1,2-Trichloroethylene

RN: 79-01-6**MP (°C):** -87**MW:** 131.39**BP (°C):** 86.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.372E-03	1.100E+00	20	M133	1 0 0 0 2	
9.654E-03	1.268E+00	20	P041	1 0 0 0 1	
8.372E-03	1.100E+00	20	P046	1 0 0 0 0	
7.603E-03	9.990E-01	25	A094	1 0 0 0 1	
1.120E-02	1.472E+00	25	B173	2 0 2 2 2	
8.363E-03	1.099E+00	25	G056	1 0 0 0 2	
8.372E-03	1.100E+00	25	M037	1 1 0 0 1	
1.040E-02	1.366E+00	25	M342	1 0 1 1 2	
8.372E-03	1.100E+00	25	M368	1 0 0 0 1	
8.363E-03	1.099E+00	25	N034	1 0 0 0 1	
3.032E-02	3.984E+00	25	N309	1 0 0 0 1	sic
5.656E-03	7.431E-01	30	M311	1 1 2 2 2	
9.274E-03	1.219E+00	37	P041	1 0 0 0 1	
8.363E-03	1.099E+00	ns	O006	0 0 0 0 1	

47. C₂HCl₃O.H₂O

Chloral (monhydrate)

Chloral-hydrat

RN: 302-17-0**MP (°C):** 57.0**MW:** 165.40**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E+00	3.400E+02	0	F300	1 0 0 0 2	
4.837E+00	8.000E+02	11.30	F300	1 0 0 0 2	
5.629E+00	9.310E+02	38.10	F300	1 0 0 0 2	
4.794E+00	7.930E+02	rt	D021	0 0 1 1 2	

48. C₂HCl₃O₂

Trichloroacetic acid

TCA

RN: 76-03-9

MP (°C): 57.5

MW: 163.39

BP (°C): 196.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.338E+00	5.455E+02	25	B185	0 0 0 0 0	
5.685E+00	9.289E+02	25	B200	1 0 0 0 2	
2.146E+00	3.506E+02	25	F018	1 0 0 0 1	
4.024E+00	6.575E+02	25	K040	1 2 1 2 2	
1.000E+01	1.634E+03	ns	M163	0 0 0 0 0	EFG
2.146E+00	3.506E+02	ns	N013	0 0 0 0 1	

49. C₂HCl₅

Pentachloroethane

Pentachloro-ethane

Pentalin

Pentachlorethane

Ethane pentachloride

RN: 76-01-7

MP (°C): -29

MW: 202.30

BP (°C): 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.322E-03	4.698E-01	20	V009	1 0 0 0 1	
2.470E-03	4.998E-01	25	G056	1 0 0 0 2	
2.472E-03	5.000E-01	25	M037	1 1 0 0 1	
2.373E-03	4.800E-01	ns	H123	0 0 0 0 0	
2.322E-03	4.698E-01	ns	O006	0 0 0 0 1	

50. C₂H₂

Acetylene

Acetylén

RN: 74-86-2

MP (°C): -81

MW: 26.04

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.796E-02	2.030E+00	0	F300	1 0 0 0 2	<i>sic</i>
4.609E-02	1.200E+00	20	F300	1 0 0 0 2	<i>sic</i>
1.862E+01	4.848E+02	25	M101	1 0 0 0 2	
1.959E-02	5.100E-01	60	F300	1 0 0 0 1	<i>sic</i>

51. C₂H₂Br₄

sym-Tetrabromoethane

1,1,2,2-Tetrabrom-aethan

Acetylene tetrabromide

1,1,2,2-Tetrabromoethane

Tetrabromoacetylene

RN: 79-27-6**MP (°C):** 0**MW:** 345.67**BP (°C):** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-03	6.500E-01	30	F300	1 0 0 0 1	
1.879E-03	6.496E-01	30	O006	1 0 0 0 1	

52. C₂H₂Cl₂

Vinylidene chloride

1,1-Dichloroethylene

RN: 75-35-4**MP (°C):** -122.0**MW:** 96.94**BP (°C):** 31.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.470E-02	2.394E+00	15	D086	1 0 2 2 1	
2.624E-02	2.544E+00	17	D086	1 0 2 2 2	
4.126E-03	4.000E-01	20	M133	1 0 0 0 2	
4.126E-03	4.000E-01	20	P046	1 0 0 0 0	
2.572E-02	2.494E+00	20.5	D086	1 0 2 2 1	
2.316E-02	2.245E+00	25	D086	1 0 2 2 2	
2.470E-02	2.394E+00	28.5	D086	1 0 2 2 1	
2.624E-02	2.544E+00	29.5	D086	1 0 2 2 2	
2.302E-02	2.232E+00	30	M311	1 1 2 2 2	
2.264E-02	2.195E+00	38.5	D086	1 0 2 2 1	
2.162E-02	2.096E+00	45	D086	1 0 2 2 1	
2.367E-02	2.295E+00	51	D086	1 0 2 2 1	
2.162E-02	2.096E+00	55	D086	1 0 2 2 1	
2.470E-02	2.394E+00	60	D086	1 0 2 2 1	
2.316E-02	2.245E+00	65	D086	1 0 2 2 2	
3.034E-02	2.941E+00	71	D086	1 0 2 2 2	
2.572E-02	2.494E+00	74.5	D086	1 0 2 2 1	
3.034E-02	2.941E+00	81	D086	1 0 2 2 2	
3.803E-02	3.686E+00	85.5	D086	1 0 2 2 1	
3.598E-02	3.488E+00	90.5	D086	1 0 2 2 1	

53. C₂H₂Cl₂

cis-Acetylene dichloride
cis-1,2-Dichloroethylene
cis-Dichlorethylene

RN: 156-59-2 **MP (°C):** -80
MW: 96.94 **BP (°C):** 60

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.610E-02	3.500E+00	25	M037	1 1 0 0 1	

54. C₂H₂Cl₂

trans-Acetylene dichloride
trans-1,2-Dichloroethylene
trans-Dichlorethylene

RN: 156-60-5 **MP (°C):** -50
MW: 96.94 **BP (°C):** 48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.499E-02	6.300E+00	25	M037	1 1 0 0 1	

55. C₂H₂Cl₃As

Chlorovinyldichloroarsine
 Chlorvinylarsin-dichlorid

RN: 541-25-3 **MP (°C):**
MW: 207.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-03	5.000E-01	20	F300	1 0 0 0 0	

56. C₂H₂Cl₄

1,1,1,2-Tetrachloroethane
 Ethane, 1,1,1,2-tetrachloro-
 F 130α
 TCA
 HCC 130α

RN: 630-20-6 **MP (°C):** -44
MW: 167.85 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.141E-03	1.199E+00	0	V009	1 0 0 0 2	
6.487E-03	1.089E+00	20	V009	1 0 0 0 2	
1.723E-02	2.892E+00	25	G056	1 0 0 0 2	
<1.66E-02	<2.79E+00	25.50	O005	2 0 2 2 1	
6.843E-03	1.149E+00	35	V009	1 0 0 0 2	
7.438E-03	1.248E+00	50	V009	1 0 0 0 2	

57. C₂H₂Cl₄

1,1,2,2-Tetrachloroethane
sym-Tetrachloroethane

RN: 79-34-5 **MP (°C):** -36
MW: 167.85 **BP (°C):** 146.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.924E-02	3.230E+00	20	C094	1 0 0 0 2	
1.758E-02	2.951E+00	23.5	S171	2 1 2 2 2	
1.770E-02	2.971E+00	25	B173	2 0 2 2 2	
1.782E-02	2.991E+00	25	F050	1 0 0 0 0	
1.728E-02	2.900E+00	25	M037	1 1 0 0 1	
1.737E-02	2.915E+00	30	M311	1 1 2 2 2	

58. C₂H₂O₄

Oxalic acid

Oxalsaeure

RN: 144-62-7 **MP (°C):** 189
MW: 90.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.683E-01	3.316E+01	0	C066	1 0 1 1 2	
3.665E-01	3.300E+01	0	L041	1 0 0 1 1	
3.756E-01	3.382E+01	0	M043	1 0 0 0 1	
4.907E-01	4.418E+01	4.99	A339	0 0 0 0 0	
6.287E-01	5.660E+01	10	M043	1 0 0 0 1	
5.912E-01	5.323E+01	9.99	A339	0 0 0 0 0	
7.752E-01	6.979E+01	14.99	A339	0 0 0 0 0	
7.441E-01	6.700E+01	15	F066	2 2 2 2 1	
7.464E-01	6.720E+01	15	F300	1 0 0 0 2	
7.775E-01	7.000E+01	15	L041	1 0 0 1 1	
9.468E-01	8.524E+01	19.99	A339	0 0 0 0 0	
9.219E-01	8.300E+01	20	F066	2 2 2 2 1	
9.219E-01	8.300E+01	20	F300	1 0 0 0 1	
9.552E-01	8.600E+01	20	L041	1 0 0 1 1	
9.636E-01	8.676E+01	20	M043	1 0 0 0 1	
8.836E-01	7.956E+01	20	M171	1 0 0 0 1	
1.146E+00	1.032E+02	24.99	A339	0 0 0 0 0	
1.088E+00	9.800E+01	25	F066	2 2 2 2 1	
1.378E+00	1.240E+02	25	F317	2 1 1 1 2	
2.480E+00	2.233E+02	25	H084	1 0 0 0 2	
1.190E+00	1.071E+02	25	H430	0 0 0 0 0	
2.409E+00	2.169E+02	25	K040	1 0 2 1 2	
1.317E+00	1.186E+02	29.99	A339	0 0 0 0 0	
1.407E+00	1.266E+02	30	M043	1 0 0 0 2	
1.623E+00	1.461E+02	34.99	A339	0 0 0 0 0	
1.710E+00	1.540E+02	35	L041	1 0 0 1 2	
1.903E+00	1.713E+02	39.99	A339	0 0 0 0 0	

(continued)

58. C₂H₂O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.973E+00	1.776E+02	40	M043	1 0 0 0 2	
2.199E+00	1.979E+02	44.99	A339	0 0 0 0 0	
2.527E+00	2.275E+02	49.99	A339	0 0 0 0 0	
2.150E+00	1.935E+02	50	C066	1 0 1 1 2	
2.821E+00	2.540E+02	50	L041	1 0 0 1 2	
2.867E+00	2.581E+02	54.99	A339	0 0 0 0 0	
3.121E+00	2.810E+02	59.99	A339	0 0 0 0 0	
3.410E+00	3.070E+02	60	M043	1 0 0 0 2	
3.661E+00	3.296E+02	64.99	A339	0 0 0 0 0	
4.121E+00	3.710E+02	65	L041	1 0 0 1 2	
3.583E+00	3.226E+02	80	C066	1 0 1 1 2	
5.084E+00	4.577E+02	80	M043	1 0 0 0 2	
6.059E+00	5.455E+02	90	F300	1 0 0 0 2	

59. C₂H₂O₄.2H₂O

Oxalic acid dihydrate

Ethanedioic acid, dihydrate

RN: 6153-56-6 MP (°C): 101
 MW: 126.07 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.443E-02	1.820E+00	23	C038	2 2 2 2 0	EFG, 0.1N HCl
1.070E-02	1.349E+00	30	C038	2 2 2 2 0	EFG, 0.1N HCl
7.234E-03	9.120E-01	35	C038	2 2 2 2 0	EFG, 0.1N HCl

60. C₂H₃Br₃O

2,2,2-Tribromoethanol

2,2,2-Tribrom-aethanol

RN: 75-80-9 MP (°C): 80
 MW: 282.77 BP (°C): 92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-01	3.410E+01	40	F300	1 0 0 0 2	

61. C₂H₃Cl

Vinyl chloride

Chloroethylene

RN: 75-01-4**MP (°C):** -153.0**MW:** 62.50**BP (°C):** -13.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-04	6.000E-02	10	M133	1 0 0 0 1	<i>sic</i>
9.600E-04	6.000E-02	10	P046	1 0 0 0 0	<i>sic</i>
1.506E-01	9.411E+00	15	D086	1 0 2 2 1	
1.576E-01	9.852E+00	16	D086	1 0 2 2 2	
1.081E-01	6.754E+00	20	N034	1 0 0 0 1	
1.451E-01	9.067E+00	20.5	D086	1 0 2 2 2	
<1.76E-02	<1.10E+00	25	I310	0 0 0 0 0	
1.396E-01	8.723E+00	26	D086	1 0 2 2 1	
1.411E-01	8.821E+00	29.5	D086	1 0 2 2 1	
1.490E-01	9.312E+00	35	D086	1 0 2 2 1	
1.411E-01	8.821E+00	41	D086	1 0 2 2 1	
1.396E-01	8.723E+00	46.5	D086	1 0 2 2 1	
6.717E-03	4.198E-01	50	M065	0 0 2 1 1	
1.506E-01	9.411E+00	55	D086	1 0 2 2 1	
1.459E-01	9.116E+00	65	D086	1 0 2 2 1	
1.553E-01	9.705E+00	72.5	D086	1 0 2 2 1	
1.584E-01	9.901E+00	80	D086	1 0 2 2 2	
1.772E-01	1.108E+01	85	D086	1 0 2 2 2	

62. C₂H₃Cl₂NO₂

1,1-Dichloro-1-nitroethane

Dichlornitroethane

Ethide

RN: 594-72-9**MP (°C):****MW:** 143.96**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.456E-02	4.975E+00	20	C121	1 0 0 0 0	unit assumed, <i>sic</i>
1.732E-02	2.494E+00	20	M061	1 0 0 0 1	

63. C₂H₃Cl₃

1,1,1-Trichloroethane

1,1,1-Trichloroethane

Trichloroethane

1,1,1-Trichloroethane

RN: 71-55-6

MP (°C): -35

MW: 133.41

BP (°C): 74.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-02	1.587E+00	0	V009	1 0 0 0 2	
1.342E-02	1.790E+00	3.5	C094	1 0 0 0 2	
1.019E-02	1.360E+00	20	C094	1 0 1 0 2	
3.358E-02	4.480E+00	20	G056	1 0 0 0 2	
3.598E-03	4.800E-01	20	M133	1 0 0 0 2	
9.895E-03	1.320E+00	20	M368	1 0 0 0 1	
3.598E-03	4.800E-01	20	P046	1 0 0 0 0	
9.882E-03	1.318E+00	20	V009	1 0 0 0 2	
8.797E-03	1.174E+00	23.5	S171	2 1 2 2 2	
5.244E-03	6.995E-01	25	A094	1 0 0 0 0	
1.000E-02	1.334E+00	25	B173	2 0 2 2 2	
3.284E-02	4.381E+00	25	N309	1 0 0 0 1	sic
9.732E-03	1.298E+00	25	O006	1 0 0 0 1	
3.597E-03	4.798E-01	30	M311	1 1 2 2 2	
9.433E-03	1.258E+00	35	V009	1 0 0 0 2	
9.583E-03	1.278E+00	50	V009	1 0 0 0 2	
5.397E-03	7.200E-01	ns	H123	0 0 0 0 0	

64. C₂H₃Cl₃

1,1,2-Trichloroethane

1,1,2-β-Trichloroethane

RN: 79-00-5

MP (°C): -37

MW: 133.41

BP (°C): 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.477E-02	4.638E+00	0	V009	1 0 0 0 2	
3.254E-02	4.341E+00	20	V009	1 0 0 0 2	
3.804E-02	5.074E+00	25	C119	2 2 2 2 2	
3.298E-02	4.400E+00	25	M037	1 1 0 0 1	
3.272E-02	4.365E+00	30	M311	1 1 2 2 2	
3.417E-02	4.559E+00	35	V009	1 0 0 0 2	
3.967E-02	5.292E+00	55	V009	1 0 0 0 2	

65. C₂H₃FO₂

Fluoroacetic acid

Essigsaeurefluorid

RN: 144-49-0

MP (°C):

MW: 78.04

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.407E-04	5.000E-02	20	F300	1 0 0 0 0	

66. C₂H₃N

Acetonitrile

Acetonitril

RN: 75-05-8

MP (°C): -45

MW: 41.05

BP (°C): 81.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.95E+01	>8.00E+02	25	B019	1 0 1 2 0	

67. C₂H₃N

Methylisocyanide

Methyl-isocyanid

RN: 593-75-9

MP (°C):

MW: 41.05

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.217E+00	9.100E+01	15	F300	1 0 0 0 1	

68. C₂H₃NS

Methyl isothiocyanate

Isothiocyanatomethane

RN: 556-61-6

MP (°C): 35

MW: 73.12

BP (°C): 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-01	7.600E+00	20	M161	1 0 0 0 1	
1.032E-01	7.543E+00	20	O300	1 0 0 0 1	
1.085E-01	7.937E+00	20	P081	1 0 0 0 0	

69. C₂H₄

Ethylene
Ethene

RN: 74-85-1 **MP (°C):** -169
MW: 28.05 **BP (°C):** 102

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.129E+00	2.000E+02	0	R028	0 0 0 0 0	
3.240E+00	9.091E+01	25	R028	0 0 0 0 0	
3.187E+00	8.942E+01	30	C116	0 0 0 0 0	

70. C₂H₄BrCl

Ethylene chlorobromide
1-Bromo-2-chloroethane

RN: 107-04-0 **MP (°C):** -17
MW: 143.42 **BP (°C):** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.778E-02	6.853E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>

71. C₂H₄Br₂

1,2-Dibromoethane
Ethylene dibromide
Curafume

Haltox
1,2-Dibromoethane
RN: 106-93-4 **MP (°C):** 9.97
MW: 187.87 **BP (°C):** 131.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.777E-02	3.339E+00	0	V009	1 0 0 0 2	
2.078E-02	3.905E+00	15	G029	1 0 2 2 2	
1.874E-02	3.520E+00	20	C094	1 0 1 0 2	
2.279E-02	4.282E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>
1.794E-02	3.370E+00	20	G080	1 0 0 0 1	
2.300E-02	4.321E+00	20	M312	1 0 0 0 1	
1.592E-02	2.991E+00	20	P081	1 0 0 0 0	
2.142E-02	4.024E+00	20	V009	1 0 0 0 2	
2.210E-02	4.153E+00	25	O006	1 0 0 0 2	
2.294E-02	4.310E+00	30	F300	1 0 0 0 2	
2.284E-02	4.292E+00	30	G029	1 0 2 2 2	
2.279E-02	4.282E+00	30	M061	1 0 0 0 1	
2.289E-02	4.300E+00	30	M161	1 0 0 0 1	
2.390E-02	4.490E+00	35	V009	1 0 0 0 2	
2.817E-02	5.292E+00	50	V009	1 0 0 0 2	

72. C₂H₄ClNO

Acetohydroxamic acid chloride

Acethydroximsaeure-chlorid

2-Chloroacetamide

Chloroacetamide

Chloressigsaeureamid

Essigsaeure-*N*-chloramid

RN: 79-07-2 MP (°C): 119.5

MW: 93.51 BP (°C): 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.624E-01	9.000E+01	24	F300	1 0 0 0 0	

73. C₂H₄ClNO₂

1-Chloro-1-nitroethane

1-Chloronitroethane

RN: 598-92-5 MP (°C):

MW: 109.51 BP (°C): 124

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.638E-02	3.984E+00	20	C121	1 0 0 0 0	unit assumed, <i>sic</i>
3.638E-02	3.984E+00	20	M061	1 0 0 0 0	

74. C₂H₄Cl₂

Ethylidene chloride

1,1-Dichloraethan

1,1-Dichloroethane

RN: 75-34-3 MP (°C): -97

MW: 98.96 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-02	6.600E+00	0	F300	1 0 0 0 1	
6.629E-02	6.560E+00	0	H101	2 0 0 0 2	
5.967E-02	5.905E+00	0	V009	1 0 0 0 2	
5.558E-02	5.500E+00	20	F300	1 0 0 0 1	
5.558E-02	5.500E+00	20	H101	2 0 0 0 2	
5.087E-02	5.035E+00	20	V009	1 0 0 0 2	
5.110E-02	5.057E+00	25	G038	1 2 2 2 2	
5.110E-02	5.057E+00	25	G053	2 2 2 1 2	
5.457E-02	5.400E+00	30	F300	1 0 0 0 1	
4.885E-02	4.834E+00	30	M300	1 1 2 2 2	
4.637E-02	4.589E+00	30	M311	1 1 2 2 2	
5.397E-02	5.341E+00	30	N034	1 0 0 0 2	
4.847E-02	4.797E+00	35	V009	1 0 0 0 2	
5.217E-02	5.163E+00	50	V009	1 0 0 0 2	

75. C₂H₄Cl₂

Ethylene dichloride

1,2-Dichloraethan

RN: 107-06-2

MP (°C): -35

MW: 98.96

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.095E-02	9.000E+00	0	F300	1 0 0 0 0	
9.317E-02	9.220E+00	0	H101	2 0 0 0 2	
9.232E-02	9.136E+00	0	L103	1 0 0 0 2	unit assumed
8.745E-02	8.654E+00	0	V009	1 0 0 0 2	
8.735E-02	8.645E+00	15	G029	1 0 2 2 2	
8.539E-02	8.450E+00	20	C094	1 0 1 0 2	
8.716E-02	8.625E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>
8.716E-02	8.625E+00	20	D052	1 1 0 0 1	
8.716E-02	8.625E+00	20	G056	1 0 0 0 2	
8.781E-02	8.690E+00	20	H101	2 0 0 0 2	
8.706E-02	8.615E+00	20	L103	1 0 0 0 2	unit assumed
8.706E-02	8.615E+00	20	M061	1 0 0 0 2	
8.616E-02	8.527E+00	20	M062	1 0 0 0 1	
8.892E-02	8.800E+00	20	M133	1 0 0 0 2	
8.716E-02	8.625E+00	20	O006	1 0 0 0 1	
8.892E-02	8.800E+00	20	P046	1 0 0 0 0	
8.507E-02	8.419E+00	20	V009	1 0 0 0 2	
8.070E-02	7.986E+00	25	B173	2 0 2 2 2	
1.060E-01	1.049E+01	25	C119	2 2 2 2 2	
8.690E-02	8.600E+00	25	F300	1 0 0 0 2	
8.740E-02	8.649E+00	25	G038	1 2 2 2 2	
8.740E-02	8.649E+00	25	G053	2 1 2 1 2	
8.488E-02	8.400E+00	25	M037	1 1 0 0 1	
9.013E-02	8.920E+00	30	G029	1 0 2 2 1	
8.954E-02	8.861E+00	30	L103	1 0 0 0 2	unit assumed
3.543E-02	3.506E+00	30	M311	1 1 2 2 2	
8.964E-02	8.871E+00	35	V009	1 0 0 0 2	
1.030E-01	1.019E+01	56	V009	1 0 0 0 2	
8.716E-02	8.625E+00	72	B197	0 0 0 0 0	at bp of 72 °C
5.927E-02	5.865E+00	89.3	B197	0 0 0 0 0	at bp of 89.3 °C
4.327E-02	4.282E+00	92.3	B197	0 0 0 0 0	at bp of 92.3 °C
3.324E-02	3.289E+00	94	B197	0 0 0 0 0	at bp of 94 °C
1.312E-02	1.298E+00	98	B197	0 0 0 0 0	at bp of 98 °C
4.345E-02	4.300E+00	rt	M161	0 0 0 0 1	

76. C₂H₄F₂

1,1-Difluoroethane

Ethylidene fluoride

RN: 75-37-6

MP (°C): -117

MW: 66.05

BP (°C): -24.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.132E-02	5.371E+00	0	M065	0 0 2 1 2	

77. C₂H₄N₂O₂

Oxamide

Oxalsaeure-diamid

RN: 471-46-5**MP (°C):****MW:** 88.07**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.201E-03	3.700E-01	7.30	F300	1 0 0 0 1	
7.040E-02	6.200E+00	100	F300	1 0 0 0 1	

78. C₂H₄N₄

Amitrole

3-Amino-1,2,4-triazole

3-Amino-*s*-triazole

ATA

Aminotriazole

RN: 61-82-5**MP (°C):** 159.0**MW:** 84.08**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.602E+00	2.188E+02	23	M061	1 0 0 0 1	
2.602E+00	2.188E+02	25	B185	0 0 0 0 0	
2.602E+00	2.188E+02	25	B200	1 0 0 0 1	
2.602E+00	2.188E+02	25	I310	0 0 0 0 0	
3.330E+00	2.800E+02	25	M161	1 0 0 0 2	
2.602E+00	2.188E+02	ns	B100	0 0 0 0 1	
3.162E+00	2.659E+02	ns	M163	0 0 0 0 0	EFG

79. C₂H₄N₄

Dicyanodiamide

Dicyandiamid

Dicyandiamide

RN: 461-58-5**MP (°C):** 210**MW:** 84.08**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.526E-01	1.283E+01	0	M043	1 0 0 0 1	
2.218E-01	1.865E+01	10	M043	1 0 0 0 1	
2.617E-01	2.200E+01	13	F300	1 0 0 0 1	
3.688E-01	3.101E+01	20	M043	1 0 0 0 1	
4.876E-01	4.100E+01	25	F300	1 0 0 0 1	
4.717E-01	3.966E+01	25.0	H037	1 2 2 1 2	
5.663E-01	4.762E+01	30	M043	1 0 0 0 1	
8.565E-01	7.201E+01	39.9	H037	1 2 2 1 2	
8.606E-01	7.236E+01	40	M043	1 0 0 0 1	
1.255E+00	1.055E+02	49.8	H037	1 2 2 1 2	

(continued)

79. C₂H₄N₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.899E+00	1.597E+02	60	M043	1 0 0 0 1	
1.878E+00	1.579E+02	60.1	H037	1 2 2 1 2	
2.236E+00	1.880E+02	60.10	F300	1 0 0 0 2	
2.978E+00	2.504E+02	74.5	H037	1 2 2 1 2	
3.275E+00	2.754E+02	80	M043	1 0 0 0 1	
1.492E-01	1.254E+01	.0	H037	1 2 2 1 2	

80. C₂H₄N₄O₂S₂

2-Amino-1,3,4-thiadiazole-5-sulfonamide
 5-Amino-1,3,4-thiadiazol-2-sulfonamide
 5-Amino-1,3,4-thiadiazole-2-sulfonamide
 CL 5343

Tio-urasin

RN: 14949-00-9 MP (°C):
 MW: 180.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-02	4.739E+00	15	K024	1 2 1 1 2	

81. C₂H₄O₂

Acetic acid glacial
 Acetic acid
 Essigsaeure

RN: 64-19-7 MP (°C): 16.7
 MW: 60.05 BP (°C): 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.004E+01	6.029E+02	25	H084	1 0 0 0 2	

82. C₂H₄O₂

Methyl formate
 Methyl methanoate
 Formic acid methyl ester

RN: 107-31-3 MP (°C): -99.8
 MW: 60.05 BP (°C): 32

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+3.80E+00	+2.28E+02	ns	S460	0 0 0 0 0	

83. C₂H₄O₃

Glycolic acid

Glykolsaeure

RN: 79-14-1**MP (°C):** 80**MW:** 76.05**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.084E+00	4.627E+02	6.99	A340	0 0 0 0 0	
6.913E+00	5.258E+02	10.89	A340	0 0 0 0 0	
7.894E+00	6.004E+02	20.69	A340	0 0 0 0 0	
8.015E+00	6.096E+02	24.99	A340	0 0 0 0 0	
8.168E+00	6.212E+02	30.09	A340	0 0 0 0 0	
8.296E+00	6.309E+02	35.99	A340	0 0 0 0 0	
8.400E+00	6.388E+02	39.99	A340	0 0 0 0 0	
8.533E+00	6.489E+02	47.99	A340	0 0 0 0 0	
8.536E+00	6.492E+02	48.99	A340	0 0 0 0 0	
8.654E+00	6.582E+02	54.99	A340	0 0 0 0 0	
8.721E+00	6.632E+02	59.49	A340	0 0 0 0 0	
8.808E+00	6.698E+02	64.49	A340	0 0 0 0 0	
8.866E+00	6.743E+02	69.99	A340	0 0 0 0 0	
8.932E+00	6.793E+02	74.99	A340	0 0 0 0 0	
8.968E+00	6.820E+02	79.89	A340	0 0 0 0 0	
9.016E+00	6.857E+02	84.49	A340	0 0 0 0 0	
9.043E+00	6.877E+02	88.09	A340	0 0 0 0 0	

84. C₂H₅Br

Bromoethane

Ethyl bromide

Aethylbromid

RN: 74-96-4**MP (°C):** -119**MW:** 108.97**BP (°C):** 38.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.792E-02	1.067E+01	0	H101	2 0 0 0 2	
8.810E-02	9.600E+00	17.5	F001	1 0 1 2 2	
8.810E-02	9.600E+00	17.5	S006	1 0 0 0 2	
8.259E-02	9.000E+00	20	F300	1 0 0 0 0	
8.388E-02	9.140E+00	20	H101	2 0 0 0 2	
8.185E-02	8.920E+00	20	H127	1 0 0 0 0	
8.127E-02	8.856E+00	30	V009	1 0 0 0 1	

85. C₂H₅Cl

Ethyl chloride
Aethylchlorid
Chloroethane
Monochloroethane

RN: 75-00-3 **MP (°C):** -139.0
MW: 64.52 **BP (°C):** 12.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.975E-02	4.500E+00	0	M037	1 1 0 0 1	
6.898E-02	4.450E+00	0	V009	1 0 0 0 2	
7.865E-02	5.074E+00	20	G056	1 0 0 0 2	
8.846E-02	5.707E+00	20	N034	1 0 0 0 2	
8.900E-02	5.742E+00	ns	F001	0 0 1 2 2	
8.433E-02	5.440E+00	ns	R028	0 0 0 0 0	

86. C₂H₅I

Iodoethane
Ethyl iodide
Aethyliodid
Iodaethan

RN: 75-03-6 **MP (°C):** -108
MW: 155.97 **BP (°C):** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.828E-02	4.410E+00	0	H101	2 0 0 0 2	
2.571E-02	4.010E+00	20	F300	1 0 0 0 2	
2.584E-02	4.030E+00	20	H101	2 0 0 0 2	
2.510E-02	3.915E+00	20	M171	1 0 0 0 2	
2.510E-02	3.915E+00	22.5	F001	1 0 1 2 2	
2.510E-02	3.915E+00	22.5	S006	1 0 0 0 2	
2.580E-02	4.024E+00	30	G029	1 0 2 2 2	
2.661E-02	4.150E+00	30	H101	2 0 0 0 2	
2.580E-02	4.023E+00	30	V009	1 0 0 0 2	

87. C₂H₅N

Ethylenimine
Aethylenimin
Aziridine
Ethyleneimine
Dimethyleneimine

RN: 151-56-4 **MP (°C):** -78
MW: 43.07 **BP (°C):** 56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.117E-01	9.116E+00	20	P315	0 0 0 0 0	

88. C₂H₅NO

Acetamide

Acetamid

RN: 60-35-5

MP (°C): 81.0

MW: 59.07

BP (°C): 222.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.021E+01	6.030E+02	.3	F300	1 0 0 0 2	
8.342E+00	4.927E+02	0	M022	1 0 0 0 2	
9.816E+00	5.798E+02	0	M043	1 0 0 0 2	
1.077E+01	6.364E+02	10	M043	1 0 0 0 2	
1.165E+01	6.880E+02	20	F300	1 0 0 0 2	
9.691E+00	5.724E+02	20	M022	1 0 0 0 2	
1.180E+01	6.970E+02	20	M043	1 0 0 0 2	
1.194E+01	7.050E+02	24.50	F300	1 0 0 0 2	
3.386E+01	2.000E+03	25	I310	0 0 0 0 0	
1.280E+01	7.561E+02	30	M043	1 0 0 0 2	
1.093E+01	6.455E+02	40	M022	1 0 0 0 2	
1.379E+01	8.148E+02	40	M043	1 0 0 0 2	
1.208E+01	7.138E+02	60	M022	1 0 0 0 2	
1.515E+01	8.947E+02	60	M043	1 0 0 0 2	
8.358E+00	4.937E+02	rt	D021	0 0 1 1 2	

89. C₂H₅NO₂

Glycine

Glycin

Glycocoll

RN: 56-40-6

MP (°C): 245

MW: 75.07

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E+00	1.252E+02	0	D018	2 2 2 1 2	
1.656E+00	1.243E+02	0	M043	1 0 0 0 2	
1.905E+00	1.430E+02	10	C347	0 0 0 0 0	EFG
2.032E+00	1.525E+02	10	M043	1 0 0 0 2	
3.025E+00	2.271E+02	15	D349	2 1 1 2 2	
1.710E+00	1.284E+02	15	G081	1 0 1 1 2	
3.009E+00	2.259E+02	20	B032	1 2 2 2 2	
2.336E+00	1.754E+02	20	C347	0 0 0 0 0	EFG
3.180E+00	2.387E+02	20	D349	2 1 1 2 2	
2.447E+00	1.837E+02	20	M043	1 0 0 0 2	
2.616E+00	1.964E+02	21	P045	1 0 2 1 2	
2.127E+00	1.597E+02	22.9	Y412	0 0 0 0 0	
2.741E+00	2.058E+02	24.99	C404	2 1 2 2 1	
3.316E+00	2.489E+02	25	B032	1 2 2 2 2	
2.885E+00	2.166E+02	25	C018	0 0 0 0 0	
2.700E-03	2.027E-01	25	C405	2 1 2 2 2	intrinsic zwit

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89. C₂H₅NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.329E+00	2.499E+02	25	D016	1 0 0 0 2	
2.691E+00	2.020E+02	25	D018	2 2 2 1 2	
2.663E+00	1.999E+02	25	D041	1 0 0 0 2	
3.325E+00	2.496E+02	25	D349	2 1 1 2 2	
2.886E+00	2.166E+02	25	E015	1 2 1 1 2	
2.660E+00	1.997E+02	25	F300	1 0 0 0 2	
2.664E+00	2.000E+02	25	G092	2 1 1 1 1	
2.664E+00	2.000E+02	25	G315	0 0 0 0 0	
2.526E+00	1.897E+02	25	K031	2 1 2 1 2	
2.886E+00	2.166E+02	25	M024	1 2 0 1 2	
3.334E+00	2.503E+02	25	M029	2 2 2 2 2	
2.760E+00	2.072E+02	25	N001	0 0 0 0 0	EFG
2.900E+00	2.177E+02	25	N012	2 0 2 1 2	
2.544E+00	1.910E+02	25	O316	1 0 1 2 2	
2.664E+00	2.000E+02	25	O316	1 0 1 2 2	
2.715E+00	2.038E+02	25	O317	1 0 1 2 2	
3.330E+00	2.500E+02	25.1	N024	0 0 0 0 0	
3.352E+00	2.516E+02	25.1	N025	0 0 0 0 0	
3.342E+00	2.509E+02	25.1	N026	0 0 0 0 0	
2.673E+00	2.006E+02	25.1	N027	1 1 2 2 2	
2.220E+00	1.667E+02	25.3	Y412	0 0 0 0 0	
3.144E+00	2.360E+02	27	D036	0 0 0 0 0	
3.074E+00	2.308E+02	27	D036	0 0 0 0 0	
2.312E+00	1.736E+02	29.2	Y412	0 0 0 0 0	
3.630E+00	2.725E+02	29.80	B032	1 2 2 1 2	
2.737E+00	2.054E+02	30	C347	0 0 0 0 0	EFG
2.832E+00	2.126E+02	30	M043	1 0 0 0 1	
3.106E+00	2.332E+02	34.99	C404	2 1 2 2 1	
2.491E+00	1.870E+02	36.8	Y412	0 0 0 0 0	
2.578E+00	1.935E+02	38.2	Y412	0 0 0 0 0	
3.109E+00	2.334E+02	40	C347	0 0 0 0 0	EFG
3.305E+00	2.481E+02	40	M043	1 0 0 0 1	
3.538E+00	2.656E+02	44.99	C404	2 1 2 2 1	
2.749E+00	2.063E+02	45.5	Y412	0 0 0 0 0	
3.547E+00	2.662E+02	50	C347	0 0 0 0 0	EFG
3.816E+00	2.865E+02	50	D018	2 2 2 1 2	
3.745E+00	2.811E+02	50	F300	1 0 0 0 2	
3.921E+00	2.943E+02	60	C347	0 0 0 0 0	EFG
4.134E+00	3.103E+02	60	M043	1 0 0 0 1	
4.215E+00	3.164E+02	70	C347	0 0 0 0 0	EFG
4.863E+00	3.650E+02	75	D018	2 2 2 1 2	
4.693E+00	3.523E+02	75	D041	1 0 0 0 2	
4.693E+00	3.523E+02	75	F300	1 0 0 0 2	
4.517E+00	3.390E+02	80	C347	0 0 0 0 0	EFG
4.836E+00	3.631E+02	80	M043	1 0 0 0 1	
4.753E+00	3.568E+02	90	C347	0 0 0 0 0	EFG
4.911E+00	3.686E+02	100	C347	0 0 0 0 0	EFG
5.353E+00	4.018E+02	100	F300	1 0 0 0 2	

(continued)

89. C₂H₅NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.485E+00	4.118E+02	100	M043	1 0 0 0 1	
5.353E+00	4.018E+02	99.99	P349	0 0 0 0 0	
1.612E+00	1.210E+02	—	C347	0 0 0 0 0	EFG
6.661E+00	5.000E+02	ns	D072	0 0 0 0 0	
4.499E+00	3.377E+02	rt	D021	0 0 1 1 2	

90. C₂H₅NO₂

Nitroethane

Nitroetan

RN: 79-24-3

MP (°C): -50

MW: 75.07

BP (°C): 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.736E-01	4.306E+01	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>
6.404E-01	4.807E+01	25	M346	2 1 1 1 2	

91. C₂H₅NO₂

Methyl carbamate

Carbamidsaeure-methyl ester

Methyl urethane

RN: 598-55-0

MP (°C): 52

MW: 75.07

BP (°C): 177

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.125E+00	6.850E+02	11	F300	1 0 0 0 2	
9.119E+00	6.845E+02	11	I314	0 0 0 0 0	
9.200E+00	6.906E+02	15.50	F001	1 0 1 0 2	
5.462E+00	4.100E+02	15.50	F300	1 0 0 0 1	

92. C₂H₅NO₂

Glycolamide

2-Hydroxyacetamide

2-Hydroxyacetimidic acid

Glycolic amide

Glycolic acid amide

RN: 598-42-5

MP (°C):

MW: 75.07

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.509E+00	4.135E+02	25	M008	1 0 0 0 2	

93. C₂H₅NS

Thiacetamide

Thioessigsaeureamid

Thioacetamide

Acetothioamide

Ethanethioamide

RN: 62-55-5**MP (°C):** 113**MW:** 75.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.865E+00	1.402E+02	25	I310	0 0 0 0 0	

94. C₂H₅N₂H₂O

Ethyleneimine (dihydrate)

Aziridine (dihydrate)

RN: 151-56-4**MP (°C):****MW:** 79.10**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.840E-02	5.411E+00	20	P315	0 0 0 0 0	

95. C₂H₅N₃O₂

Methylnitrosourea

MNU

Nitrosomethylurea

RN: 684-93-5**MP (°C):** 123**MW:** 103.08**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	1.443E+01	24	M031	1 1 1 1 1	
1.413E-01	1.456E+01	ns	R424	0 0 0 0 0	

96. C₂H₅N₃O₂

Biuret

Carbamylurea

RN: 108-19-0**MP (°C):****MW:** 103.08**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.164E-01	1.200E+01	0	F300	1 0 0 0 2	
1.475E-01	1.520E+01	15	F300	1 0 0 0 2	
3.104E+00	3.200E+02	106	F300	1 0 0 0 1	

97. C₂H₅N₅O₃

N-Methyl-N'-nitro-N-nitrosoguanidine

MNNG

1-Methyl-3-nitro-1-nitrosoguanidine

RN: 70-25-7 MP (°C): 118

MW: 147.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.38E-02	<4.98E+00	ns	I307	0 0 0 0 0	

98. C₂H₅O₅P

Phosphoacetic acid

Phosphor carboxymethyl-phosphonsaeure

Phosphonoacetic acid

RN: 4408-78-0 MP (°C): 144.5

MW: 140.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.799E+00	3.920E+02	0	F300	1 0 0 0 2	
2.800E+00	3.921E+02	0	N028	1 0 0 0 2	

99. C₂H₅O₅As

Arsonoacetic acid

Arsono-essigsaeure

RN: 107-38-0 MP (°C): 152

MW: 183.98 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.174E+00	4.000E+02	18	F300	1 0 0 0 1	

100. C₂H₆

Ethane

Aethan

RN: 74-84-0 MP (°C): -172

MW: 30.07 BP (°C): -88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.587E-01	7.779E+00	0	C075	1 0 1 0 1	
4.157E-03	1.250E-01	0	F300	1 0 0 0 2	
3.601E-03	1.083E-01	4.99	C115	2 0 2 2 2	
2.903E-03	8.730E-02	9.99	C115	2 0 2 2 2	
2.465E-03	7.413E-02	14.99	C115	2 0 2 2 2	

(continued)

100. C₂H₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-03	6.682E-02	19.8	G058	1 0 0 0 2	
2.129E-03	6.401E-02	19.99	C115	2 0 2 2 2	
1.929E-03	5.800E-02	20	F300	1 0 0 0 1	
1.850E-03	5.563E-02	24.99	C115	2 0 2 2 2	
2.009E-03	6.040E-02	25	M001	2 1 2 2 2	
2.009E-03	6.040E-02	25	M002	2 2 1 2 2	
1.760E-03	5.292E-02	25	M102	1 2 2 1 2	
1.620E-03	4.871E-02	29.99	C115	2 0 2 2 2	
7.981E-04	2.400E-02	60	F300	1 0 0 0 1	

101. C₂H₆O

Methyl ether

Dimethyl ether

Dimethylaether

RN: 115-10-6

MP (°C): -138

MW: 46.07

BP (°C): -23.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.476E+00	6.800E+01	18	F300	1 0 0 0 1	
5.669E+00	2.612E+02	24	M065	1 0 2 1 2	

102. C₂H₆O₂

Ethylene glycol

Glycol

1,2-Ethandiol

RN: 107-21-1

MP (°C): -13

MW: 62.07

BP (°C): 197.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.710E+00	4.165E+02	4.50	C022	1 2 0 0 2	
5.562E-01	3.452E+01	25	B004	0 0 0 0 0	

103. C₂H₆O₃S

Methyl methanesulphonate

Methyl mesylate

Methanesulfonic acid methyl ester

RN: 66-27-3

MP (°C): 20

MW: 110.13

BP (°C): 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.513E+00	1.667E+02	25	I310	0 0 0 0 0	

104. C₂H₆O₄S

Dimethyl sulfate

Sulfuric acid dimethyl ester

RN: 77-78-1 **MP (°C):** -27
MW: 126.13 **BP (°C):** 188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-01	2.800E+01	18	B078	1 0 0 0 1	
2.159E-01	2.724E+01	18	D049	1 2 0 0 1	

105. C₂H₇N

Ethylamine

Aethylamin

RN: 75-04-7 **MP (°C):** -81
MW: 45.08 **BP (°C):** 16.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.686E-02	1.211E+00	25	B004	0 0 0 0 0	

106. C₂H₇NO₃S

Taurine

Taurin

RN: 107-35-7 **MP (°C):** 328
MW: 125.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.999E-01	3.754E+01	0	M043	1 0 0 0 1	
4.523E-01	5.660E+01	10	M043	1 0 0 0 1	
4.842E-01	6.060E+01	12	F300	1 0 0 0 2	
3.919E-01	4.905E+01	15	G081	1 0 1 1 2	
6.448E-01	8.070E+01	20	F300	1 0 0 0 2	
6.463E-01	8.088E+01	20	M043	1 0 0 0 1	
4.700E-01	5.882E+01	24	D031	1 0 0 0 2	
7.580E-01	9.486E+01	25	D041	1 0 0 0 2	
8.815E-01	1.103E+02	30	M043	1 0 0 0 2	
1.149E+00	1.438E+02	40	M043	1 0 0 0 2	
1.719E+00	2.151E+02	60	M043	1 0 0 0 2	
1.985E+00	2.484E+02	70	F300	1 0 0 0 2	
2.105E+00	2.634E+02	75	D041	1 0 0 0 2	
2.217E+00	2.775E+02	80	M043	1 0 0 0 2	
2.506E+00	3.137E+02	100	M043	1 0 0 0 2	

107. C₂H₇O₂As

Cacodylic acid

Dimethylarsinsaeure

Kakodylsaeure

Arsine oxide, hydroxydimethyl-

Cacodylic acid

RN: 75-60-5**MP (°C):** 195**MW:** 138.00**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.899E+00	4.001E+02	20	B200	1 0 0 0 2	
3.287E+00	4.536E+02	22	B185	0 0 0 0 0	
3.290E+00	4.540E+02	22	F300	1 0 0 0 2	
4.961E+00	6.845E+02	25	D305	1 0 0 0 2	
1.449E+01	2.000E+03	25	M161	1 0 0 0 0	

108. C₂H₇As

Ethylarsine

Aethylarsin

Arsen

RN: 593-59-9**MP (°C):****MW:** 106.00**BP (°C):** 36

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-03	1.300E-01	19	F300	1 0 0 0 1	

109. C₂Cl₂F₄

1,2-Dichlorotetrafluoroethane

CFC-114

sym-Dichlorotetrafluoroethane

Halon 242

1,2-Dichloro-1,1,2,2-tetrafluoroethane

Cryofluorane

RN: 76-14-2**MP (°C):** -94**MW:** 170.92**BP (°C):** 3.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.605E-04	1.300E-01	25	R048	0 0 0 0 0	

110. C₂Cl₃F₃

1,1,2-Trichloro-1,2,2-trifluoroethane

Freon 113

Fluorocarbon 113

Halocarbon 113

RN: 76-13-1 MP (°C): -36.4

MW: 187.38 BP (°C): 47.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.071E-04	1.700E-01	25	R048	0 0 0 0 0	

111. C₂Cl₄

Tetrachloroethylene

Ethylene tetrachloride

Perchloroethylene

Tetrachloroethene

Tetrachloro-ethylene

PERC

RN: 127-18-4 MP (°C): -22

MW: 165.83 BP (°C): 121

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-03	2.000E-01	20	C094	1 0 1 0 2	
1.206E-03	2.000E-01	20	C121	0 0 0 0 0	unit assumed, <i>sic</i>
9.045E-04	1.500E-01	20	M133	1 0 0 0 2	
9.045E-04	1.500E-01	20	P046	1 0 0 0 0	
9.044E-04	1.500E-01	25	A094	1 0 0 0 1	
2.920E-03	4.842E-01	25	B173	2 0 2 2 2	
1.206E-03	2.000E-01	25	C119	2 2 2 2 2	
2.412E-03	4.000E-01	25	F071	1 1 2 1 2	
9.044E-04	1.500E-01	25	G056	1 0 0 0 2	
9.045E-04	1.500E-01	25	M037	1 1 0 0 1	
9.045E-04	1.500E-01	25	M368	1 0 0 0 1	
9.044E-04	1.500E-01	25	N034	1 0 0 0 1	
2.412E-03	4.000E-01	ns	M344	0 0 0 0 2	
9.044E-04	1.500E-01	ns	O006	0 0 0 0 1	

112. C₂Cl₆

Hexachloroethane

1,1,1,2,2,2-Hexachloroethane

Avlothane

Distopin

Distopan

Distokal

RN: 67-72-1**MP (°C):** 187**MW:** 236.74**BP (°C):** 186.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.253E-05	7.700E-03	20	M339	2 2 2 2 1	
2.112E-04	5.000E-02	22.3	M037	1 1 0 0 0	
1.148E-04	2.718E-02	ns	R427	0 0 0 0 0	

113. C₂N₂

Cyanogen

Dicyan

RN: 460-19-5**MP (°C):****MW:** 52.04**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.572E+01	8.182E+02	20	F300	1 0 0 0 1	

114. C₂N₄S₂

Cyanogen azidodithiocarbonate

RN:**MP (°C):****MW:** 144.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-02	1.500E+00	0	A055	0 0 0 0 2	

115. C₂N₆S₄

Thioperoxydicarbonic diazide

Azidoschwefel-kohlenstoff

Azidocarbonicdisulfide

RN: 148832-09-1**MP (°C):****MW:** 236.32**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.269E-03	3.000E-01	25	F300	1 0 0 0 0	

116. C₃H₂Cl₂N₂O₂

1,3-Dichlorohydantoin

2,4-Imidazolidinedione, 1,3-dichloro-

RN: 2958-99-8 **MP (°C):****MW:** 168.97 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.114E-02	6.951E+00	20	B080	1 0 1 1 0	
8.171E-02	1.381E+01	40	B080	1 0 1 1 1	

117. C₃H₂N₂

Malononitrile

Malonsaeure-dinitril

RN: 109-77-3 **MP (°C):** 32**MW:** 66.06 **BP (°C):** 218.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E+00	1.176E+02	20	F300	1 0 0 0 2	
1.778E+00	1.175E+02	ns	R424	0 0 0 0 0	

118. C₃H₂N₂O₃

Parabanic acid

Parabansaeure

RN: 120-89-8 **MP (°C):****MW:** 114.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.945E-01	4.500E+01	8	F300	1 0 0 0 1	

119. C₃H₃Cl₃O₃

β,β,β-Trichlorolactic acid

β,β,β-Trichlor-milchsaeure

RN: 599-01-9 **MP (°C):****MW:** 193.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E+00	4.380E+02	25	F300	1 0 0 0 2	

120. C₃H₃N

Acrylonitrile
Propenitrile

RN: 107-13-1 **MP (°C):** -83.5
MW: 53.06 **BP (°C):** 77.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.266E+00	6.716E+01	0	D046	0 0 0 0 0	
1.266E+00	6.716E+01	0	D046	2 2 0 0 1	EFG
1.282E+00	6.803E+01	20	D046	0 0 0 0 0	
1.282E+00	6.803E+01	20	D046	2 2 0 0 1	EFG
1.298E+00	6.890E+01	25	D046	2 2 0 0 1	EFG
1.298E+00	6.890E+01	25	D046	0 0 0 0 0	
1.298E+00	6.890E+01	25	L096	1 2 0 2 1	
1.413E+00	7.500E+01	25	M161	1 0 0 0 1	
1.315E+00	6.977E+01	28	D046	2 2 0 0 1	EFG
1.347E+00	7.149E+01	36	D046	2 2 0 0 1	EFG
1.364E+00	7.236E+01	39	D046	2 2 0 0 1	EFG
1.388E+00	7.365E+01	41	D046	2 2 0 0 2	EFG
1.508E+00	8.004E+01	49	D046	2 2 0 0 1	EFG
1.508E+00	8.004E+01	53	D046	2 2 0 0 1	EFG
1.540E+00	8.173E+01	59	D046	2 2 0 0 1	EFG
1.603E+00	8.509E+01	63	D046	2 2 0 0 1	EFG
1.760E+00	9.338E+01	65	A324	2 2 2 1 2	
1.651E+00	8.759E+01	68	D046	2 2 0 0 0	EFG
1.721E+00	9.132E+01	72	D046	2 2 0 0 0	EFG
1.869E+00	9.918E+01	80	D046	2 2 0 0 0	EFG
1.974E+00	1.047E+02	85	D046	2 2 1 1 0	EFG
2.124E+00	1.127E+02	90	D046	2 2 1 1 0	EFG

121. C₃H₃NOS₂

Rhodanine
Rhodanin

RN: 141-84-4 **MP (°C):** 170
MW: 133.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.689E-02	2.250E+00	25	F300	1 0 0 0 2	

122. C₃H₃N₃O₃

Cyanuric acid

Cyanursaeure

Isocyanuric acid

Isocyanursaeure

RN: 108-80-5**MP (°C):****MW:** 129.08**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-02	2.969E+00	2	B193	1 2 0 0 1	
3.874E-02	5.000E+00	20	F300	1 0 0 0 0	
2.009E-02	2.593E+00	25	B384	0 0 0 0 0	

123. C₃H₃N₃O₃

Cyamelide

Cyamelid

RN: 462-02-2**MP (°C):****MW:** 129.08**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.747E-04	1.000E-01	15	F300	1 0 0 0 0	

124. C₃H₃N₃S₃

Trithiocyanuric acid

s-Triazine-2,4,6-trithiol

Trimercapto-s-triazine

RN: 638-16-4**MP (°C):****MW:** 177.27**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.354E-03	2.399E-01	25	B384	0 0 0 0 0	

125. C₃H₄

Propyne

Methyl acetylene

Methylacetylene

RN: 74-99-7**MP (°C):** -101**MW:** 40.07**BP (°C):** -23.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.085E-02	3.239E+00	21	I011	1 2 2 1 2	
9.085E-02	3.640E+00	25	M001	2 1 2 2 2	
5.488E-02	2.199E+00	38	I011	1 2 2 1 1	
3.606E-02	1.445E+00	54	I011	1 2 2 1 1	
2.220E-02	8.895E-01	71	I011	1 2 2 1 1	
8.886E-03	3.560E-01	88	I011	1 2 2 1 1	

126. C₃H₄ClN₅

Desethyl simazine

Amino-2-chloro-6-ethylamino-*s*-triazine6-Chloro-*N*-ethyl-1,3,5-triazine-2,4-diamine**RN:** 1007-28-9 **MP (°C):****MW:** 145.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	1.747E-01	2	B193	1 1 0 0 0	

127. C₃H₄Cl₂

1,2-Dichloropropene

Dichloropropylene

RN: 26952-23-8 **MP (°C):****MW:** 110.97 **BP (°C):** 92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-02	2.693E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>

128. C₃H₄Cl₂*trans*-1,3-Dichloropropene1,3-Dichloropropylene (*trans*)*trans*-1,3-Dichloropropylene

1,3-Dichloropropene

RN: 542-75-6 **MP (°C):****MW:** 110.97 **BP (°C):** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.703E-03	2.999E-01	20	C121	1 0 0 0 0	unit assumed, <i>sic</i>
9.011E-03	1.000E+00	20	M161	1 0 0 0 0	
1.071E-02	1.188E+00	30	M300	1 1 2 2 2	

129. C₃H₄Cl₂*cis*-1,3-Dichloropropene1,3-Dichloropropylene (*cis*)*cis*-1,3-Dichloropropylene*cis* 1,3-Dichloro-propene*cis*-1,3-Dichloro-1-propene

(Z)-1,3-Dichloropropene

RN: 10061-01-5 **MP (°C):****MW:** 110.97 **BP (°C):** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.433E-02	2.700E+00	20	G080	1 0 0 0 1	
9.651E-03	1.071E+00	30	M300	1 1 2 2 2	
8.211E-03	9.112E-01	30	M311	1 1 2 2 2	

130. C₃H₄Cl₂*trans*-1,3-Dichloro-propene*trans*-1,3-Dichloro-1-propene

(E)-1,3-Dichloro-1-propene

E-1,3-Dichloropropene

RN: 10061-02-6 MP (°C):

MW: 110.97 BP (°C): 111

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.523E-02	2.800E+00	20	G080	1 0 0 0 1	

131. C₃H₄Cl₂O₂

Dalapon

 α,α -Dichlor-propionsaeure

RN: 75-99-0 MP (°C):

MW: 142.97 BP (°C): 187.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.511E+00	5.020E+02	25	M161	1 0 0 0 2	
3.511E+00	5.020E+02	ns	K138	0 0 0 0 1	

132. C₃H₄N₂O

Cyanoacetamide

Cyanessigsaeure-amid

RN: 107-91-5 MP (°C):

MW: 84.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.546E+00	1.300E+02	20	F300	1 0 0 0 1	

133. C₃H₄N₂O₂

Hydantoin

2,4-Imidazolidinedione

RN: 461-72-3 MP (°C): 220

MW: 100.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.944E+00	2.946E+02	100	F300	1 0 0 0 2	
3.970E-01	3.973E+01	ns	M025	0 2 0 1 2	

134. C₃H₄N₂O₃S

2-Imidazole sulfonic acid

Imidazol-sulfosaeure-(2)

RN: 53744-47-1 **MP (°C):**
MW: 148.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.009E-01	7.420E+01	20	F300	1 0 0 0 2	

135. C₃H₄N₄O₂

Ammelide

2,4-Dihydroxy-6-amino-1,3,5-triazine

RN: 645-93-2 **MP (°C):**
MW: 128.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	7.685E-02	2	B193	1 2 0 0 0	

136. C₃H₄O

Acrolein

2-Propenal

Acrylaldehyde

RN: 107-02-8 **MP (°C):** -88.0
MW: 56.06 **BP (°C):** 52.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.690E+00	4.872E+02	0	B111	1 0 0 1 1	Quinol as a stabilizer
3.764E+00	2.110E+02	20	F300	1 0 0 0 2	
3.071E+00	1.722E+02	20	M161	1 0 0 0 1	
8.522E+00	4.778E+02	32.50	B111	1 0 0 1 2	Quinol as a stabilizer
8.429E+00	4.726E+02	44.40	B111	1 0 0 1 2	Quinol as a stabilizer
8.339E+00	4.675E+02	50	B111	1 0 0 1 2	Quinol as a stabilizer
8.288E+00	4.647E+02	53	B111	1 0 0 1 2	Quinol as a stabilizer
7.889E+00	4.423E+02	74.50	B111	1 0 0 1 2	Quinol as a stabilizer
7.338E+00	4.114E+02	82	B111	1 0 0 1 2	Quinol as a stabilizer
7.013E+00	3.932E+02	84	B111	1 0 0 1 2	Quinol as a stabilizer
6.597E+00	3.699E+02	87.80	B111	1 0 0 1 2	Quinol as a stabilizer
6.417E+00	3.598E+02	88	B111	1 0 0 1 2	Quinol as a stabilizer
5.096E+00	2.857E+02	ns	B185	0 0 0 0 0	
3.567E+00	2.000E+02	ns	B200	0 0 0 0 0	

137. C₃H₄O₄

Malonic acid

Acide malonique

Malonsaeure

RN: 141-82-2**MP (°C):** 135**MW:** 104.06**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.645E+00	3.793E+02	0	F300	1 0 0 0 2	
5.871E+00	6.110E+02	0	L041	1 0 0 1 2	
4.990E+00	5.192E+02	0	M043	1 0 0 0 2	
5.871E+00	6.110E+02	0	M051	1 0 0 0 2	
4.743E+00	4.936E+02	4.99	A339	0 0 0 0 0	
5.427E+00	5.648E+02	10	K077	1 2 2 2 2	average of 3
5.395E+00	5.614E+02	10	M043	1 0 0 0 2	
4.888E+00	5.087E+02	9.99	A339	0 0 0 0 0	
5.034E+00	5.238E+02	14.99	A339	0 0 0 0 0	
5.608E+00	5.836E+02	15	K077	1 2 2 2 2	
6.746E+00	7.020E+02	15	L041	1 0 0 1 2	
6.746E+00	7.020E+02	15	M051	1 0 0 0 2	
5.728E+00	5.961E+02	18	K077	1 2 2 2 2	
5.198E+00	5.409E+02	19.99	A339	0 0 0 0 0	
7.063E+00	7.350E+02	20	L041	1 0 0 1 2	
5.811E+00	6.047E+02	20	M043	1 0 0 0 2	
4.067E+00	4.232E+02	20	M171	1 0 0 0 2	
2.670E+00	2.778E+02	20	S006	1 0 0 0 2	
5.928E+00	6.169E+02	24	K077	1 2 2 2 2	
5.354E+00	5.571E+02	24.99	A339	0 0 0 0 0	
4.221E+00	4.393E+02	25	F300	1 0 0 0 2	
5.990E+00	6.233E+02	25	K077	1 2 2 2 2	
7.332E+00	7.630E+02	25	M051	1 0 0 0 2	
5.494E+00	5.717E+02	29.99	A339	0 0 0 0 0	
6.178E+00	6.429E+02	30	M043	1 0 0 0 2	
5.638E+00	5.867E+02	34.99	A339	0 0 0 0 0	
7.938E+00	8.260E+02	35	L041	1 0 0 1 2	
5.800E+00	6.035E+02	39.99	A339	0 0 0 0 0	
6.530E+00	6.795E+02	40	M043	1 0 0 0 2	
5.913E+00	6.153E+02	44.99	A339	0 0 0 0 0	
6.028E+00	6.273E+02	49.99	A339	0 0 0 0 0	
8.898E+00	9.260E+02	50	L041	1 0 0 1 2	
8.898E+00	9.260E+02	50	M051	1 0 0 0 2	
6.895E+00	7.175E+02	53	K077	1 2 2 2 2	
6.182E+00	6.433E+02	54.99	A339	0 0 0 0 0	
6.328E+00	6.585E+02	59.99	A339	0 0 0 0 0	
7.158E+00	7.449E+02	60	M043	1 0 0 0 2	
6.451E+00	6.713E+02	64.99	A339	0 0 0 0 0	
9.831E+00	1.023E+03	65	L041	1 0 0 1 2	
7.878E+00	8.198E+02	80	M043	1 0 0 0 2	
8.267E+00	8.603E+02	93	K077	1 2 2 2 2	
8.554E+00	8.901E+02	100	M043	1 0 0 0 2	
9.610E+00	1.000E+03	132	K077	1 2 2 2 2	
1.441E+01	1.500E+03	ns	D072	0 0 0 0 1	

138. C₃H₅Br

Allyl bromide

3-Bromopropene

RN: 106-95-6 **MP (°C):** -119
MW: 120.98 **BP (°C):** 71.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.170E-02	3.835E+00	25	M342	1 0 1 1 2	

139. C₃H₅Bvr₂Cl

1,2-Dibromo-3-chloropropane

1-Chloro-2,3-dibromopropane

Nemagon

RN: 96-12-8 **MP (°C):**
MW: 236.34 **BP (°C):** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.204E-03	1.230E+00	20	G080	1 0 0 0 1	
4.227E-03	9.990E-01	20	P081	1 0 0 0 0	
4.227E-03	9.990E-01	ns	I316	0 0 0 0 0	
4.227E-03	9.990E-01	ns	M061	0 0 0 0 0	
4.231E-03	1.000E+00	rt	M161	0 0 0 0 0	

140. C₃H₅Cl

Allyl chloride

3-Chloro-1-propene

RN: 107-05-1 **MP (°C):** -134
MW: 76.53 **BP (°C):** 44

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.687E-02	3.587E+00	20	G056	1 0 0 0 2	
1.305E-02	9.990E-01	ns	N034	0 0 0 0 0	

141. C₃H₅ClO

Chloroacetone

1-Chloro-2-propanone

Chloraceton

RN: 78-95-5 **MP (°C):** -44.5
MW: 92.53 **BP (°C):** 119.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.924E-01	8.257E+01	ns	N034	0 0 0 0 0	

142. C₃H₅ClO

Epichlorohydrin

Epichloridrina

RN: 106-89-8

MP (°C): -25.6

MW: 92.53

BP (°C): 117.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.577E-01	6.086E+01	0	L061	1 2 2 1 2	
6.615E-01	6.121E+01	10	L061	1 2 2 1 2	
6.501E-01	6.015E+01	20	I313	0 0 0 0 0	
6.692E-01	6.191E+01	30.20	L061	1 2 2 1 2	
7.568E-01	7.003E+01	52	L061	1 2 2 1 2	
8.421E-01	7.792E+01	65	L061	1 2 2 1 2	
9.232E-01	8.542E+01	72	L061	1 2 2 1 2	
1.024E+00	9.478E+01	80.20	L061	1 2 2 1 2	

143. C₃H₅Cl₂NO₂

1,1-Dichloro-1-nitropropane

Propane, 1,1-dichloro-1-nitro-

RN: 595-44-8

MP (°C):

MW: 157.98

BP (°C): 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.149E-02	4.975E+00	20	C121	1 0 0 0 0	unit assumed, sic

144. C₃H₅Cl₃

1,2,3-Trichloropropane

Allyl trichloride

Trichlorohydrin

Glycerol trichlorohydrin

RN: 96-18-4

MP (°C): -14

MW: 147.43

BP (°C): 156

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-02	1.900E+00	ns	H123	0 0 0 0 0	

145. C₃H₅IO₂

β-Iodopropionic acid

β-Iod-propionsäure

RN: 141-76-4

MP (°C): 81.5

MW: 199.98

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.715E-01	7.430E+01	25	F300	1 0 0 0 2	

146. C₃H₅N

Propionitrile

Propionsaeure-nitril

n-Propionitrile

RN: 107-12-0 **MP (°C):** -93
MW: 55.08 **BP (°C):** 97

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.151E-02	3.388E+00	25	B004	0 0 0 0 0	

147. C₃H₅N

Ethyl isocyanide

Ethane, isocyano-

RN: 624-79-3 **MP (°C):**
MW: 55.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.814E-02	9.990E-01	ns	L055	0 0 0 0 1	

148. C₃H₅NO

Acrylamide

2-Propenamide

RN: 79-06-1 **MP (°C):** 84
MW: 71.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.299E+00	3.056E+02	0	M147	0 2 1 1 0	EFG
4.690E+00	3.333E+02	10	M147	0 2 1 1 0	EFG
5.220E+00	3.711E+02	20	M147	0 2 1 1 0	EFG
5.695E+00	4.048E+02	30	M147	0 2 1 1 0	EFG
6.075E+00	4.318E+02	40	M147	0 2 1 1 0	EFG
6.253E+00	4.444E+02	50	M147	0 2 1 1 0	EFG
6.625E+00	4.709E+02	60	M147	0 2 1 1 0	EFG
7.034E+00	5.000E+02	80	M147	0 2 1 1 0	EFG

149. C₃H₅NO₃

Formylglycine

N-Formyl glycine

RN: 2491-15-8 **MP (°C):**
MW: 103.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.849E+00	1.906E+02	25	M024	1 2 0 1 2	
1.849E+00	1.906E+02	ns	M025	0 2 0 1 2	

150. C₃H₅N₃O

Ethynitrosocyanamide

ENC

RN: 38434-77-4

MP (°C):

MW: 99.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	1.387E+01	24	M031	1 1 1 1 1	

151. C₃H₅N₃O₉

Nitroglycerin

Nitroglycerol

RN: 55-63-0

MP (°C): 13.5

MW: 227.09

BP (°C): 256

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.629E-03	1.278E+00	15	L063	2 0 1 1 2	
7.926E-03	1.800E+00	20	F300	1 0 0 0 1	
6.069E-03	1.378E+00	20	L063	2 0 1 1 2	
5.504E-03	1.250E+00	25	P312	0 0 0 0 0	
6.595E-03	1.498E+00	30	L063	2 0 1 1 2	
7.342E-03	1.667E+00	40	L063	2 0 1 1 2	
8.570E-03	1.946E+00	50	L063	2 0 1 1 2	
1.041E-02	2.364E+00	60	L063	2 0 1 1 2	
1.265E-02	2.872E+00	70	L063	2 0 1 1 2	
1.518E-02	3.448E+00	80	L063	2 0 1 1 2	

152. C₃H₅N₅O

Ammeline

Ammelin

RN: 645-92-1

MP (°C):

MW: 127.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	7.626E-02	2	B193	1 1 0 0 0	
5.901E-04	7.500E-02	23	F300	1 0 0 0 1	
2.486E-03	3.160E-01	100	F300	1 0 0 0 2	

153. C₃H₆

Cyclopropane
Trimethylene

RN: 75-19-4 **MP (°C):** -127
MW: 42.08 **BP (°C):** -33

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.461E-02	1.036E+00	5.05	Z008	2 1 2 2 2	at 97.26 kPa
1.281E-02	5.390E-01	20	R060	0 0 0 0 0	
1.754E-02	7.382E-01	21	I017	1 2 2 1 2	at 16.9 psia
1.103E-02	4.640E-01	25	R060	0 0 0 0 0	
9.315E-03	3.920E-01	30	R060	0 0 0 0 0	
8.983E-03	3.780E-01	31	R060	0 0 0 0 0	
7.723E-03	3.250E-01	35	R060	0 0 0 0 0	
1.083E-02	4.557E-01	38	I017	1 2 2 1 2	at 17.0 psia
6.844E-03	2.880E-01	39	R060	0 0 0 0 0	
5.917E-03	2.490E-01	45	R060	0 0 0 0 0	
8.386E-03	3.529E-01	71	I017	1 2 2 1 2	at 19.9 psia
3.999E-03	1.683E-01	104	I017	1 2 2 1 2	at 24.9 psia
5.896E+00	2.481E+02	ns	R028	0 0 0 0 0	

154. C₃H₆

Propylene
Methyl ethylene
Propene

RN: 115-07-1 **MP (°C):** -185
MW: 42.08 **BP (°C):** -48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.139E-02	9.000E-01	0	F300	1 0 0 0 1	
7.553E-03	3.178E-01	21	A052	1 1 1 2 2	smoothed
7.842E-03	3.300E-01	25	F300	1 0 0 0 1	
4.753E-03	2.000E-01	25	M001	2 1 2 2 2	
4.221E-03	1.776E-01	38	A052	1 1 1 2 1	smoothed
2.333E-03	9.818E-02	54	A052	1 1 1 2 1	smoothed
1.500E-03	6.312E-02	71	A052	1 1 1 2 1	smoothed
7.222E-04	3.039E-02	88	A052	1 1 1 2 1	smoothed

155. C₃H₆BrCl

1-Bromo-3-chloropropane
w-Chlorobromopropane
3-Bromopropyl chloride
3-Chloro-1-bromopropane

RN: 109-70-6 **MP (°C):** -58.9
MW: 157.44 **BP (°C):** 143.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-02	2.236E+00	25	M342	1 0 1 1 2	

156. C₃H₆BrNO₄

Bronopol

2-Bromo-2-nitropropane-1,3-diol

RN: 52-51-7 **MP (°C):** 130
MW: 199.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E+00	2.000E+02	22	M161	1 0 0 0 1	

157. C₃H₆Br₂

Trimethylene bromide

1,3-Dibromopropane

RN: 109-64-8 **MP (°C):** -36
MW: 201.90 **BP (°C):** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.406E-03	1.697E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>

158. C₃H₆ClNO₂

1-Chloro-1-nitropropane

Propane, 1-chloro-1-nitro-

RN: 600-25-9 **MP (°C):**
MW: 123.54 **BP (°C):** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.424E-02	7.937E+00	20	C121	1 0 0 0 0	unit assumed, <i>sic</i>
4.027E-02	4.975E+00	20	M061	1 0 0 0 0	

159. C₃H₆ClNO₂

1-Chloro-2-nitropropane

Propane, 1-chloro-2-nitro-

RN: 37809-02-2 **MP (°C):**
MW: 123.54 **BP (°C):** 174

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.424E-02	7.937E+00	20	M061	1 0 0 0 0	

160. C₃H₆Cl₂

Propylene dichloride

1,2-Dichlor-propan

1,2-Dichloropropane

Propylene chloride

Dichloropropane

RN: 78-87-5**MP (°C):** -100.3**MW:** 112.99**BP (°C):** 96.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.160E-02	3.570E+00	20	C094	1 0 1 0 2	
2.383E-02	2.693E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>
2.390E-02	2.700E+00	20	F300	1 0 0 0 1	
2.390E-02	2.700E+00	20	M037	1 1 0 0 1	
2.383E-02	2.693E+00	20	M061	1 0 0 0 1	
2.295E-02	2.593E+00	20	M062	1 0 0 0 1	
2.390E-02	2.700E+00	20	M161	1 0 0 0 1	
2.500E-02	2.825E+00	20	M312	1 0 0 0 1	
2.383E-02	2.693E+00	20	N034	1 0 0 0 1	
2.478E-02	2.800E+00	25	F300	1 0 0 0 1	
2.480E-02	2.802E+00	25	G038	1 2 2 2 2	
2.480E-02	2.802E+00	25	G053	2 1 2 1 2	
2.295E-02	2.593E+00	25	G056	1 0 0 0 2	
2.142E-02	2.420E+00	30	M300	1 1 2 2 2	
1.831E-02	2.069E+00	30	M311	1 1 2 2 2	

161. C₃H₆Cl₂

1,3-Dichloropropane

1,3-Dichlor-propan

RN: 142-28-9**MP (°C):** -99**MW:** 112.99**BP (°C):** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.559E-02	2.892E+00	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>
2.416E-02	2.730E+00	25	F300	1 0 0 0 2	
2.430E-02	2.746E+00	25	G038	1 2 2 2 2	
2.430E-02	2.746E+00	25	G053	2 1 2 1 2	
9.027E-03	1.020E+00	30	M311	1 1 2 2 2	

162. C₃H₆Cl₂O

1,3-Dichloro-2-propanol

1,3-Dichlor-propanol-(2)

RN: 96-23-1**MP (°C):** -4**MW:** 128.99**BP (°C):** 174.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.675E-01	9.900E+01	19	F300	1 0 0 0 1	
6.984E-01	9.008E+01	19	N034	1 0 0 0 1	
1.124E+00	1.450E+02	72	F300	1 0 0 0 2	

163. C₃H₆N₂O₂

Malonic acid diamide

Malonsaeure-diamid

Malonamide

Malonodiamide

Propanediamide

RN: 108-13-4**MP (°C):** 170**MW:** 102.09**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.513E-01	7.670E+01	8	F300	1 0 0 0 2	
7.830E-03	7.994E-01	ns	L055	0 0 0 0 1	

164. C₃H₆N₂O₂

Methylglyoxime

Methylglyoxim

RN: 1804-15-5**MP (°C):****MW:** 102.09**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.506E-01	4.600E+01	26	F300	1 0 0 0 1	
7.444E-01	7.600E+01	40	F300	1 0 0 0 1	

165. C₃H₆N₂O₂

Methylnitrosoacetamide

MNA

RN: 7417-67-6**MP (°C):****MW:** 102.09**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-01	1.736E+01	24	M031	1 1 1 1 1	

166. C₃H₆N₂O₂

1-Acetylurea

Acetylharnstoff

RN: 591-07-1**MP (°C):** 218**MW:** 102.09**BP (°C):** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-01	1.300E+01	15	F300	1 0 0 0 1	

167. C₃H₆N₂O₃

Hydantoic acid

N-(Carboxymethyl)urea

N-Carbamoylglycine

Carbamoylglycine

Glycoluric acid

RN: 462-60-2**MP (°C):****MW:** 118.09**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.549E-01	3.010E+01	20	F300	1 0 0 0 2	
3.290E-01	3.885E+01	25	M024	1 2 0 1 2	
3.290E-01	3.885E+01	ns	M025	0 2 0 1 2	

168. C₃H₆N₂O₇

Glycerol 1,2-dinitrate

1,2,3-Propanetriol 1,2-dinitrate

1,2-Dinitroglycerol

RN: 131287-51-9**MP (°C):****MW:** 182.09**BP (°C):** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.386E-01	6.165E+01	20	D013	1 0 1 1 2	

169. C₃H₆N₂O₇

Glycerol 1,3-dinitrate

Glycerol- α,α' -dinitrateGlycerin- α,α' -dinitrate**RN:** 623-87-0**MP (°C):** 26**MW:** 182.09**BP (°C):** 116

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.993E-01	7.270E+01	20	D013	1 0 1 1 2	

170. C₃H₆N₂S

Ethylenethiourea

Mercaptoimidazoline

Mercozen

RN: 96-45-7**MP (°C):** 203**MW:** 102.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.919E-01	1.961E+01	30	I310	0 0 0 0 0	
8.082E-01	8.257E+01	60	I310	0 0 0 0 0	
2.991E+00	3.056E+02	90	I310	0 0 0 0 0	

171. C₃H₆N₄Hg

Methylmercuridicyanodiamide

Panogen

RN: 502-39-6

MP (°C): 156

MW: 298.70

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.265E-02	2.170E+01	20	M061	1 0 0 0 2	
7.265E-02	2.170E+01	rt	M161	0 0 0 0 2	

172. C₃H₆N₆

Melamine

1,3,5-Triazine-2,4,6-triamine

Cymel

RN: 108-78-1

MP (°C):

MW: 126.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.503E-03	1.199E+00	0	M043	1 0 0 0 1	
1.000E-02	1.261E+00	2	B193	1 1 0 0 1	
1.425E-02	1.797E+00	10	M043	1 0 0 0 1	
2.561E-02	3.230E+00	19.90	C023	2 2 0 1 2	
2.135E-02	2.693E+00	20	M043	1 0 0 0 1	
3.316E-02	4.182E+00	30	M043	1 0 0 0 1	
4.651E-02	5.865E+00	34.90	C023	2 2 0 1 2	
5.590E-02	7.050E+00	40	M043	1 0 0 0 1	
8.200E-02	1.034E+01	49.80	C023	2 2 0 1 2	
1.172E-01	1.478E+01	60	M043	1 0 0 0 1	
1.325E-01	1.672E+01	64.10	C023	2 2 0 1 2	
1.836E-01	2.315E+01	74.50	C023	2 2 0 1 2	
2.160E-01	2.724E+01	80	M043	1 0 0 0 1	
2.421E-01	3.054E+01	83.50	C023	2 2 0 1 2	
3.480E-01	4.389E+01	94.80	C023	2 2 0 1 2	
3.812E-01	4.807E+01	99	C023	2 2 0 1 2	
3.776E-01	4.762E+01	100	M043	1 0 0 0 1	

173. C₃H₆N₆O₆

Cyclonite

RDX

RN: 121-82-4

MP (°C): 205

MW: 222.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	5.975E-02	25	B173	2 0 2 2 2	

174. C₃H₆O

Propylene oxide

Methyl ethylene oxide

RN: 75-56-9 **MP (°C):** -112
MW: 58.08 **BP (°C):** 34.23

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.963E+00	2.883E+02	20	I313	0 0 0 0 0	
2.544E-01	1.478E+01	20	M065	1 0 2 1 1	<i>sic</i>
6.389E+00	3.711E+02	25	I313	0 0 0 0 0	

175. C₃H₆O

Acetone

2-Propanone

Aceton

RN: 67-64-1 **MP (°C):** -94
MW: 58.08 **BP (°C):** 56.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		0	C423	0 0 0 0 0	
		4	C423	0 0 0 0 0	
		10	C423	0 0 0 0 0	

176. C₃H₆O

Propaldehyde

Propyl aldehyde

Propanal

RN: 123-38-6 **MP (°C):** -81
MW: 58.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.870E+00	1.667E+02	20	D041	1 0 0 0 0	
2.927E+00	1.700E+02	20	F300	1 0 0 0 1	
5.269E+00	3.060E+02	25	A049	1 0 0 0 2	
3.105E+00	1.803E+02	25	B060	2 0 1 1 1	
2.880E+00	1.673E+02	25	F044	1 0 0 0 2	

177. C₃H₆O₂

Propionic acid

n-Propionic acid

RN: 79-09-4 **MP (°C):** -22
MW: 74.08 **BP (°C):** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-01	2.025E+01	25	B004	0 0 0 0 0	

178. C₃H₆O₂

Ethyl formate

Ameisensaeure-ethyl ester

Formic acid ethyl ester

RN: 109-94-4 **MP (°C):** -80
MW: 74.08 **BP (°C):** 53

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.094E+00	8.108E+01	5.0	K079	1 0 0 0 2	
1.139E+00	8.437E+01	15.9	K079	1 0 0 0 2	
1.350E+00	1.000E+02	18	F300	1 0 0 0 1	
1.350E+00	1.000E+02	22	S006	1 0 0 0 2	
1.194E+00	8.848E+01	30.2	K079	1 0 0 0 2	
1.239E+00	9.178E+01	38.0	K079	1 0 0 0 2	
1.283E+00	9.507E+01	45.1	K079	1 0 0 0 2	
1.339E+00	9.918E+01	50.0	K079	1 0 0 0 2	
1.383E+00	1.025E+02	55.5	K079	1 0 0 0 2	
1.517E+00	1.124E+02	63.9	K079	1 0 0 0 2	
1.639E+00	1.214E+02	70.0	K079	1 0 0 0 2	
1.778E+00	1.317E+02	75.5	K079	1 0 0 0 2	

179. C₃H₆O₂

Methyl acetate

Essigsaeures methyl

Methylacetat

RN: 79-20-9 **MP (°C):** -98.0
MW: 74.08 **BP (°C):** 56.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.678E+00	2.725E+02	5.0	K079	1 0 0 0 2	
4.017E+00	2.976E+02	20	E002	1 0 0 0 2	
3.290E+00	2.437E+02	20	F001	1 0 1 2 2	
2.647E+00	1.961E+02	20	F300	1 0 0 0 2	
3.290E+00	2.437E+02	20	M171	1 0 0 0 2	
4.617E+00	3.420E+02	20	P040	0 0 0 0 0	
4.300E+00	3.185E+02	20	S006	1 0 0 0 1	
3.722E+00	2.757E+02	21.0	K079	1 0 0 0 2	
2.772E-02	2.054E+00	25	B004	0 0 0 0 0	<i>sic</i>
3.772E+00	2.794E+02	35.0	K079	1 0 0 0 2	
3.889E+00	2.881E+02	58.0	K079	1 0 0 0 2	
3.906E+00	2.893E+02	58.9	K079	1 0 0 0 2	
3.922E+00	2.906E+02	60.1	K079	1 0 0 0 2	
3.950E+00	2.926E+02	61.7	K079	1 0 0 0 2	
4.172E+00	3.091E+02	69.1	K079	1 0 0 0 2	
4.256E+00	3.153E+02	70.5	K079	1 0 0 0 2	
4.294E+00	3.181E+02	71.9	K079	1 0 0 0 2	
4.906E+00	3.634E+02	83.5	K079	1 0 0 0 2	
4.252E-02	3.150E+00	c	L055	0 0 0 0 2	

180. C₃H₆O₂S₃ α -Trimethylene trisulphide dioxide1,3,5-Trithiane, 1,3-dioxide, *trans*-**RN:** 60077-04-5 **MP (°C):****MW:** 170.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.817E-02	1.672E+01	25	B112	1 2 1 1 2	

181. C₃H₆O₂S₃ β -Trimethylene trisulphide dioxide1,3,5-Trithiane, 1,3-dioxide, *cis*-**RN:** 60041-48-7 **MP (°C):****MW:** 170.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.545E-01	4.334E+01	25	B112	1 2 1 1 2	

182. C₃H₆O₃

DL-Glyceraldehyde

DL-Glycerin-aldehyd

RN: 56-82-6 **MP (°C):** 145**MW:** 90.08 **BP (°C):** 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.233E-01	2.913E+01	18	D041	1 0 0 0 0	
3.242E-01	2.920E+01	18	F300	1 0 0 0 2	

183. C₃H₆O₃

Hydracrylic acid

Hydracrylsaeure

RN: 503-66-2 **MP (°C):****MW:** 90.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.998E+00	2.701E+02	25	I307	0 0 0 0 0	

184. C₃H₆O₃

s-Trioxane

1,3,5-Trioxan

RN: 110-88-3

MP (°C): 64

MW: 90.08

BP (°C): 114.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.715E+00	1.544E+02	20.00	B394	0 0 0 0 0	
1.943E+00	1.750E+02	25	F300	1 0 0 0 2	
2.033E+00	1.831E+02	25.00	B394	0 0 0 0 0	
2.403E+00	2.165E+02	30.10	B394	0 0 0 0 0	
2.741E+00	2.469E+02	34.45	B394	0 0 0 0 0	
4.187E+00	3.772E+02	43.00	B394	0 0 0 0 0	
4.462E+00	4.019E+02	44.00	B394	0 0 0 0 0	
4.606E+00	4.149E+02	44.40	B394	0 0 0 0 0	
4.826E+00	4.348E+02	45.00	B394	0 0 0 0 0	
4.816E+00	4.338E+02	45.10	B394	0 0 0 0 0	
5.355E+00	4.824E+02	46.00	B394	0 0 0 0 0	
5.311E+00	4.784E+02	46.10	B394	0 0 0 0 0	
6.401E+00	5.766E+02	47.10	B394	0 0 0 0 0	
8.161E+00	7.351E+02	47.80	B394	0 0 0 0 0	
8.534E+00	7.687E+02	48.95	B394	0 0 0 0 0	
8.741E+00	7.874E+02	50.20	B394	0 0 0 0 0	
9.095E+00	8.192E+02	55.30	B394	0 0 0 0 0	

185. C₃H₆O₃S₃

α-Trimethylene trisulphoxide

1,3,5-Trithiane, 1,3,5-trioxide, (1 α ,3 α ,5 α)-

RN: 60102-87-6 MP (°C):

MW: 186.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.184E-03	1.338E+00	25	B112	1 2 1 1 2	

186. C₃H₆O₃S₃

β-Trimethylene trisulphoxide

1,3,5-Trithiane, 1,3,5-trioxide, (1 α ,3 α ,5 β)-

RN: 60102-88-7 MP (°C):

MW: 186.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.605E-02	1.417E+01	25	B112	1 2 1 1 2	

187. C₃H₆O₃S

1,3-Propane sultone

1,2-Oxathiolane 2,2-dioxide

3-Hydroxy-1-propanesulfonic acid g-sultone

RN: 1120-71-4 **MP (°C):** 31
MW: 122.14 **BP (°C):** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.187E-01	1.000E+02	ns	I307	0 0 0 0 0	

188. C₃H₇Br

Isopropyl bromide

Isopropylbromid

RN: 75-26-3 **MP (°C):** -89
MW: 123.00 **BP (°C):** 59

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.398E-02	4.180E+00	0	H101	2 0 0 0 2	
2.340E-02	2.878E+00	18	F001	1 0 1 2 2	
2.602E-02	3.200E+00	20	F300	1 0 0 0 1	
2.585E-02	3.180E+00	20	H101	2 0 0 0 2	
2.592E-02	3.188E+00	30	V009	1 0 0 0 1	

189. C₃H₇Br

Propyl bromide

1-Bromopropane

Propylbromid

Bromopropane

RN: 106-94-5 **MP (°C):** -110
MW: 123.00 **BP (°C):** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.415E-02	2.970E+00	0	F300	1 0 0 0 2	
2.423E-02	2.980E+00	0	H101	2 0 0 0 2	
1.850E-02	2.275E+00	19.5	S006	1 0 0 0 2	
1.850E-02	2.275E+00	19.50	F001	1 0 1 0 2	
1.992E-02	2.450E+00	20	H101	2 0 0 0 2	
1.947E-02	2.394E+00	20	H127	1 0 0 0 1	
1.874E-02	2.305E+00	30	G029	1 0 2 2 2	
1.876E-02	2.307E+00	30	V009	1 0 0 0 2	
1.140E-01	1.402E+01	ns	H307	0 0 0 0 0	

190. C₃H₇BrO

3-Bromo-1-propanol

3-Bromopropanol-(1)

RN: 627-18-9

MP (°C):

MW: 139.00

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.022E+00	1.420E+02	20	F300	1 0 0 0 2	

191. C₃H₇Cl

Isopropyl chloride

2-Chloropropane

RN: 75-29-6

MP (°C): -117

MW: 78.54

BP (°C): 35

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.602E-02	4.400E+00	0	H101	2 0 0 0 2	
4.380E-02	3.440E+00	12.50	F001	1 0 1 0 2	
3.947E-02	3.100E+00	20	F300	1 0 0 0 1	
3.883E-02	3.050E+00	20	H101	2 0 0 0 2	
3.935E-02	3.090E+00	20	N034	1 0 0 0 1	
3.888E-02	3.054E+00	30	V009	1 0 0 0 1	

192. C₃H₇Cl

Chloropropane

Propyl chloride

1-Chloropropane

RN: 540-54-5

MP (°C): -123

MW: 78.54

BP (°C): 43.47

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.787E-02	3.760E+00	0	H101	2 0 0 0 2	
2.970E-02	2.333E+00	12.50	F001	1 0 1 0 2	
3.438E-02	2.700E+00	20	F300	1 0 0 0 1	
3.463E-02	2.720E+00	20	H101	2 0 0 0 2	
3.428E-02	2.693E+00	20	N034	1 0 0 0 1	
2.970E-02	2.333E+00	20	S006	1 0 0 0 2	
3.520E-02	2.765E+00	30	V009	1 0 0 0 2	

193. C₃H₇ClO

3-Chloro-1-propanol

3-Chloropropanol-(1)

RN: 627-30-5

MP (°C):

MW: 94.54

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.644E+00	2.500E+02	20	F300	1 0 0 0 1	
+2.64E+00	+2.50E+02	ns	S460	0 0 0 0 0	

194. C₃H₇I

Iodopropane

n-Propyl iodide

RN: 107-08-4

MP (°C): -101

MW: 169.99

BP (°C): 101.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.706E-03	1.140E+00	0	H101	2 0 0 0 2	
5.100E-03	8.670E-01	20	F001	1 0 1 0 2	
5.118E-03	8.700E-01	20	F300	1 0 0 0 1	
6.294E-03	1.070E+00	20	H101	2 0 0 0 2	
5.100E-03	8.670E-01	20	M171	1 0 0 0 1	
5.100E-03	8.670E-01	20	S006	1 0 0 0 1	
6.258E-03	1.064E+00	23.5	S171	2 1 2 2 2	
6.112E-03	1.039E+00	30	G029	1 0 2 2 2	
6.094E-03	1.036E+00	30	V009	1 0 0 0 1	

195. C₃H₇I

Isopropyl iodide

2-Iodopropane

RN: 75-30-9

MP (°C): -90

MW: 169.99

BP (°C): 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.824E-03	1.670E+00	0	H101	2 0 0 0 2	
8.236E-03	1.400E+00	20	F300	1 0 0 0 1	
8.236E-03	1.400E+00	20	H101	2 0 0 0 2	
7.889E-03	1.341E+00	30	V009	1 0 0 0 1	

196. C₃H₇NO₂

1-Nitropropane

n-Nitropropane

RN: 108-03-2

MP (°C): -108

MW: 89.09

BP (°C): 131.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-01	1.381E+01	20	C121	1 0 0 0 1	unit assumed, <i>sic</i>

197. C₃H₇NO₂

2-Nitropropane

Nitroisopropane

Dimethylnitromethane

RN: 79-46-9

MP (°C): -93

MW: 89.09

BP (°C): 120.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.876E-01	1.672E+01	20	C121	0 0 0 0 1	unit assumed, <i>sic</i>
1.874E-01	1.670E+01	20	F300	1 0 0 0 2	
2.376E-01	2.117E+01	20	H118	1 1 1 1 2	

198. C₃H₇NO₂ α -Alanine

Alanine

2-Aminopropanoic acid

2-Ammoniopropanoate

L-2-Aminopropionic acid

RN: 56-41-7

MP (°C): 314.5–316.5

MW: 89.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.366E+00	1.217E+02	10	C347	0 0 0 0 0	EFG
1.640E+00	1.461E+02	15	D349	2 1 1 2 2	
1.744E+00	1.554E+02	20	B032	1 2 2 1 2	
1.535E+00	1.367E+02	20	C347	0 0 0 0 0	EFG
1.780E+00	1.586E+02	20	D349	2 1 1 2 2	
1.838E+00	1.638E+02	25	B032	1 2 2 1 2	
1.590E+00	1.417E+02	25	D005	2 2 1 1 2	
1.602E+00	1.427E+02	25	D041	1 0 0 0 2	
1.870E+00	1.666E+02	25	D349	2 1 1 2 2	
1.660E+00	1.479E+02	25	E015	1 2 1 1 1	
1.595E+00	1.421E+02	25	G092	2 1 1 1 1	
1.595E+00	1.421E+02	25	G315	0 0 0 0 0	
1.654E+00	1.474E+02	25	G433	0 0 0 0 0	
1.852E+00	1.650E+02	25	J303	0 0 0 0 0	
1.600E+00	1.426E+02	25	N001	0 0 0 0 0	EFG
1.630E+00	1.452E+02	25	N012	2 0 2 1 2	
1.555E+00	1.386E+02	25	O316	1 0 1 2 2	

(continued)

198. C₃H₇NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.598E+00	1.424E+02	25	O316	1 0 1 2 2	
1.623E+00	1.446E+02	25	O317	1 0 1 2 2	
1.871E+00	1.667E+02	25.1	N024	0 0 0 0 0	
1.871E+00	1.667E+02	25.1	N026	0 0 0 0 0	
1.606E+00	1.431E+02	25.1	N027	1 1 2 2 2	
1.704E+00	1.518E+02	27	D036	0 0 0 0 0	
1.695E+00	1.510E+02	27	D036	0 0 0 0 0	
1.940E+00	1.728E+02	29.80	B032	1 2 2 1 2	
1.657E+00	1.477E+02	30	C347	0 0 0 0 0	EFG
1.956E+00	1.743E+02	30	J303	0 0 0 0 0	
1.816E+00	1.618E+02	40	C347	0 0 0 0 0	EFG
2.192E+00	1.953E+02	40	J303	0 0 0 0 0	
1.931E+00	1.720E+02	45	F300	1 0 0 0 2	
1.932E+00	1.721E+02	50	C347	0 0 0 0 0	EFG
2.430E+00	2.165E+02	50	J303	0 0 0 0 0	
2.118E+00	1.887E+02	60	C347	0 0 0 0 0	EFG
2.706E+00	2.411E+02	60	J303	0 0 0 0 0	
2.333E+00	2.078E+02	70	C347	0 0 0 0 0	EFG
2.489E+00	2.218E+02	75	D041	1 0 0 0 2	
2.504E+00	2.230E+02	80	C347	0 0 0 0 0	EFG
2.668E+00	2.377E+02	90	C347	0 0 0 0 0	EFG
2.888E+00	2.573E+02	100	C347	0 0 0 0 0	EFG
1.192E+00	1.062E+02	-	C347	0 0 0 0 0	EFG
1.587E+00	1.414E+02	rt	D021	0 0 1 1 2	

199. C₃H₇NO₂

β-Alanine

β-Alanin

RN: 107-95-9

MP (°C):

MW: 89.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E+00	3.528E+02	25	D041	1 0 0 0 2	
6.123E+00	5.455E+02	25	M024	1 2 0 1 2	

200. C₃H₇NO₂

D-Alanine

D(-)-Alanine

RN: 338-69-2

MP (°C): 292

MW: 89.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.265E+00	1.127E+02	0	M043	1 0 0 0 2	
1.396E+00	1.243E+02	10	M043	1 0 0 0 2	

(continued)

200. C₃H₇NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E+00	1.363E+02	20	D041	1 0 0 0 2	
1.531E+00	1.364E+02	20	M043	1 0 0 0 2	
1.589E+00	1.416E+02	25	D005	2 2 1 1 2	
1.680E+00	1.497E+02	30	M043	1 0 0 0 2	
1.839E+00	1.639E+02	40	M043	1 0 0 0 2	
2.194E+00	1.955E+02	60	M043	1 0 0 0 2	
2.590E+00	2.308E+02	80	M043	1 0 0 0 2	
3.049E+00	2.717E+02	100	M043	1 0 0 0 2	
3.049E+00	2.717E+02	99.99	P349	0 0 0 0 0	

201. C₃H₇NO₂

DL-Alanine

DL- α -Alanine

DL-2-Aminopropionic acid

RN: 302-72-7 MP (°C): 289

MW: 89.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+00	1.080E+02	0	D018	2 2 2 1 2	
1.212E+00	1.080E+02	0	F300	1 0 0 0 2	
1.212E+00	1.079E+02	0	M043	1 0 0 0 2	
1.361E+00	1.213E+02	10	M043	1 0 0 0 0	
1.523E+00	1.357E+02	20	M043	1 0 0 0 0	
1.557E+00	1.387E+02	21	P045	1 0 2 1 2	
1.659E+00	1.478E+02	25	C018	0 0 0 0 0	
1.596E+00	1.422E+02	25	D018	2 2 2 1 2	
1.598E+00	1.424E+02	25	D041	1 0 0 0 2	
1.607E+00	1.432E+02	25	F300	1 0 0 0 2	
1.900E+00	1.693E+02	25	J303	0 0 0 0 0	
1.530E+00	1.363E+02	25	K031	2 1 2 1 2	
2.024E+00	1.803E+02	30	J303	0 0 0 0 0	
1.704E+00	1.518E+02	30	M043	1 0 0 0 0	
2.307E+00	2.055E+02	40	J303	0 0 0 0 0	
1.894E+00	1.687E+02	40	M043	1 0 0 0 0	
2.134E+00	1.902E+02	50	D018	2 2 2 1 2	
2.106E+00	1.876E+02	50	F300	1 0 0 0 2	
2.591E+00	2.308E+02	50	J303	0 0 0 0 0	
2.954E+00	2.632E+02	60	J303	0 0 0 0 0	
2.337E+00	2.082E+02	60	M043	1 0 0 0 0	
2.733E+00	2.435E+02	75	D018	2 2 2 1 2	
2.734E+00	2.436E+02	75	D041	1 0 0 0 2	
2.714E+00	2.418E+02	75	F300	1 0 0 0 2	
2.842E+00	2.532E+02	80	M043	1 0 0 0 0	
3.431E+00	3.057E+02	100	F300	1 0 0 0 2	
3.430E+00	3.056E+02	100	M043	1 0 0 0 2	
3.432E+00	3.057E+02	99.99	P349	0 0 0 0 0	

202. C₃H₇NO₂

Lactamide

2-Hydroxypropionamide

RN: 2043-43-8 MP (°C):

MW: 89.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.779E+00	7.822E+02	25	M008	1 0 0 0 2	

203. C₃H₇NO₂

Sarcosine

Sarkosin

RN: 107-97-1 MP (°C): 208

MW: 89.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.151E-01	4.589E+01	20	D041	1 0 0 0 2	
3.367E+00	3.000E+02	20	F300	1 0 0 0 2	
4.807E+00	4.282E+02	20	P045	1 0 2 1 2	

204. C₃H₇NO₂

Urethan

Carbamidsaeure-aethyl ester

Eyethyl urethan

Urethane

Ethyl carbamate

Carbamic acid ethyl ester

RN: 51-79-6 MP (°C): 49

MW: 89.09 BP (°C): 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.918E+00	2.600E+02	11	F300	1 0 0 0 1	
5.393E+00	4.805E+02	15.5	F001	1 0 1 2 2	
2.245E+01	2.000E+03	25	I310	0 0 0 0 0	
5.074E+00	4.521E+02	25	P065	2 0 1 1 2	
1.800E+01	1.604E+03	37	H006	1 2 2 1 1	
8.901E+00	7.930E+02	40	F300	1 0 0 0 2	

205. C₃H₇NO₂S

Cysteine

2-Amino-3-mercaptopropanoic acid

RN: 3374-22-9 MP (°C): 225

MW: 121.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.773E-02	3.360E+00	20	P045	1 0 2 1 2	

206. C₃H₇NO₃

Serine

2-Amino-3-hydroxypropanoic acid

L(-)-Serin

RN: 56-45-1 **MP (°C):** 220
MW: 105.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.556E+00	1.635E+02	10.19	J417	0 0 0 0 0	
1.626E+00	1.709E+02	12.69	J417	0 0 0 0 0	
4.530E-01	4.761E+01	15	D349	2 1 1 2 2	
1.864E+00	1.959E+02	16.09	J417	0 0 0 0 0	
1.903E+00	2.000E+02	20	D041	1 0 0 0 1	
4.610E-01	4.845E+01	20	D349	2 1 1 2 2	
9.512E-01	9.997E+01	20	F300	1 0 0 0 2	
3.405E+00	3.578E+02	20.00	B032	1 2 2 1 2	<i>sic</i>
4.700E-01	4.939E+01	25	D349	2 1 1 2 2	
2.807E+00	2.950E+02	25	G315	0 0 0 0 0	<i>sic</i>
4.013E+00	4.217E+02	25	J303	0 0 0 0 0	
4.043E+00	4.249E+02	25.00	B032	1 2 2 0 2	<i>sic</i>
2.228E+00	2.342E+02	25.89	J417	0 0 0 0 0	
3.578E+00	3.760E+02	27	D036	0 0 0 0 0	
2.287E+00	2.404E+02	27.89	J417	0 0 0 0 0	
4.690E+00	4.929E+02	29.80	B032	1 2 2 1 2	<i>sic</i>
5.633E+00	5.920E+02	40	J303	0 0 0 0 0	
2.800E+00	2.943E+02	42.79	J417	0 0 0 0 0	
2.811E+00	2.954E+02	43.79	J417	0 0 0 0 0	
2.861E+00	3.007E+02	44.59	J417	0 0 0 0 0	
2.902E+00	3.050E+02	49.69	J417	0 0 0 0 0	
2.972E+00	3.124E+02	53.89	J417	0 0 0 0 0	
7.574E+00	7.960E+02	60	J303	0 0 0 0 0	

207. C₃H₇NO₃

D-Serine

D-2-Amino-3-hydroxypropanoic acid

RN: 312-84-5 **MP (°C):** 220
MW: 105.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.903E+00	2.000E+02	20	D041	1 0 0 0 0	
4.010E+00	4.214E+02	25	J303	0 0 0 0 0	
5.709E+00	6.000E+02	40	J303	0 0 0 0 0	
7.631E+00	8.020E+02	60	J303	0 0 0 0 0	

208. C₃H₇NO₃

DL-Serine

DL-2-Amino-3-hydroxypropanoic acid

RN: 302-84-1 **MP (°C):** 240
MW: 105.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.778E-01	2.920E+01	10	F300	1 0 0 0 2	
3.787E-01	3.980E+01	20	F300	1 0 0 0 2	
4.548E-01	4.780E+01	25	D041	1 0 0 0 2	
4.805E-01	5.050E+01	25	J303	0 0 0 0 0	
7.403E-01	7.780E+01	40	J303	0 0 0 0 0	
8.916E-01	9.370E+01	50	F300	1 0 0 0 2	
1.261E+00	1.325E+02	60	J303	0 0 0 0 0	
1.533E+00	1.611E+02	75	D041	1 0 0 0 2	
1.532E+00	1.610E+02	75	F300	1 0 0 0 2	
2.320E+00	2.438E+02	100	F300	1 0 0 0 2	
2.320E+00	2.438E+02	99.99	P349	0 0 0 0 0	

209. C₃H₇NO₃

DL-Isoserine

DL-Isoserin

RN: 632-12-2 **MP (°C):** 235
MW: 105.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E-01	1.530E+01	20	F300	1 0 0 0 2	

210. C₃H₇NO₅Glycerol- α -nitrateGlycerin- α -nitrate

RN: 27321-61-5 **MP (°C):**
MW: 137.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E+00	4.118E+02	15	F300	1 0 0 0 2	

211. C₃H₇N₃O₂

Glycocyamine

Guanidin-essigsaeure

Guanidineacetic acid

RN: 352-97-6 **MP (°C):** 280
MW: 117.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.825E-02	4.480E+00	15	D041	1 0 0 0 1	
3.074E-02	3.600E+00	15	F300	1 0 0 0 1	

212. C₃H₇N₃O₂

Nitrosoethylurea

N-Nitroso-N-ethylurea

RN: 759-73-9 **MP (°C):** 103
MW: 117.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.096E-01	1.283E+01	rt	I306	0 0 0 0 0	

213. C₃H₇O₅P

2-Carboxyethylphosphonic acid

3-Phosphonopropionic acid

RN: 5962-42-5 **MP (°C):**
MW: 154.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.845E+00	2.842E+02	0	N028	1 0 0 0 2	
2.129E+00	3.280E+02	20	N028	1 0 0 0 2	

214. C₃H₈

Propane

Propan

RN: 74-98-6 **MP (°C):** -187
MW: 44.10 **BP (°C):** -42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.460E-03	1.526E-01	4	K031	2 1 2 1 2	
2.472E-03	1.090E-01	10	F300	1 0 0 0 2	
2.721E-03	1.200E-01	18	M065	0 0 2 1 1	1 atm, <i>sic</i>
1.761E-03	7.765E-02	19.8	G058	1 0 0 0 2	
1.746E-03	7.700E-02	20	F300	1 0 0 0 1	
1.420E-03	6.261E-02	25	B342	1 2 1 1 1	
1.530E-03	6.747E-02	25	K031	2 1 2 1 2	
1.415E-03	6.240E-02	25	M001	2 1 2 2 2	
1.415E-03	6.240E-02	25	M002	2 1 2 2 2	
8.400E-04	3.704E-02	50	K031	2 1 2 1 2	
6.123E-04	2.700E-02	60	F300	1 0 0 0 1	

215. C₃H₈NO₅P

Glyphosate

N-(Phosphonomethyl)glycine

Bronco

RN: 1071-83-6 **MP (°C):** 230.0
MW: 169.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.097E-02	1.200E+01	25	M161	1 0 0 0 1	
5.856E-02	9.901E+00	ns	B100	0 0 0 0 0	

216. C₃H₈O

n-Propyl alcohol

Propanol

RN: 71-23-8 **MP (°C):** -127.0
MW: 60.10 **BP (°C):** 97.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.132E+00	1.882E+02	ns	L003	0 0 2 1 2	
+4.17E+00	+2.51E+02	ns	S460	0 0 0 0 0	

217. C₃H₈O

Isopropyl alcohol

2-Propanol

RN: 67-63-0 **MP (°C):** -88
MW: 60.10 **BP (°C):** 82.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.033E+00	3.025E+02	ns	L003	0 0 2 1 1	

218. C₃H₈OS₂

2,3-Dimercapto-1-propanol

Dimercaprol

RN: 59-52-9 **MP (°C):**
MW: 124.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.963E-01	7.407E+01	20	D041	1 0 0 0 0	

219. C₃H₈O₂

Methylal

Formaldehyd-dimethyl-acetal

RN: 109-87-5 **MP (°C):** -105
MW: 76.10 **BP (°C):** 41.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E+00	2.441E+02	16	B117	1 0 0 1 2	
3.022E+00	2.300E+02	20	F300	1 0 0 0 1	

220. C₃H₈O₃

Glycerol

Glycerin

RN: 56-81-5 **MP (°C):** 20
MW: 92.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.973E+00	5.501E+02	4.50	C022	1 2 0 0 2	
5.751E-01	5.296E+01	25	B004	0 0 0 0 0	

221. C₃H₉N

Propylamine

Propylamin

n-Propylamine

RN: 107-10-8 **MP (°C):** -83
MW: 59.11 **BP (°C):** 48

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.469E-02	1.459E+00	25	B004	0 0 0 0 0	

222. C₃H₉N

Trimethylamine

N,N-Dimethylmethanamine

RN: 75-50-3 **MP (°C):** -124.0
MW: 59.11 **BP (°C):** 3.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>6.77E+00	>4.00E+02	20	F300	1 0 0 0 0	
6.936E+00	4.100E+02	25	A049	1 0 0 0 2	

223. C₃H₉O₄P

Trimethyl phosphate

Phosphorsaeure-trimethyl ester

RN: 512-56-1 **MP (°C):**
MW: 140.08 **BP (°C):** 197

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.569E+00	5.000E+02	25	F300	1 0 0 0 1	
3.573E+00	5.005E+02	ns	S460	0 0 0 0 0	

224. C₃H₁₂N₆O₃

Guanidine carbonate

Guanidin-carbonat

RN: 3425-08-9 **MP (°C):** 198
MW: 180.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E+00	3.333E+02	24	F300	1 0 0 0 2	

225. C₃Cl₃N₃O₃

Trichloroisocyanuric acid

Symclosene

RN: 87-90-1 **MP (°C):** 246.5
MW: 232.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.439E-03	7.994E-01	20	B080	1 0 1 1 0	
2.311E-02	5.371E+00	40	B080	1 0 1 1 1	

226. C₃Cl₆

Hexachloropropene

Hexachloropropylene

Perchloropropene

Hexachloro-1-propene

1,1,2,3,3-Hexachloro-1-propene

1,1,2,3,3-Hexachloropropene

RN: 1888-71-7 **MP (°C):**
MW: 248.75 **BP (°C):** 209–210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.026E-04	1.499E-01	ns	S460	0 0 0 0 0	

227. C₄HI₄N

Iadol

2,3,4,5-Tetraiodpyrrol

RN: 87-58-1 **MP (°C):**
MW: 570.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.505E-04	2.000E-01	15	F300	1 0 0 0 2	

228. C₄H₂

Butadiyne

Diacetylen

RN: 460-12-8 **MP (°C):** -36.4
MW: 50.06 **BP (°C):** 10.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	1.000E-01	25	F300	1 0 0 0 0	

229. C₄H₂N₂O₄

Alloxan

Alloxane

RN: 50-71-5 **MP (°C):** 256dec
MW: 142.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.631E-02	8.000E+00	ns	D072	0 0 0 0 0	
5.623E-02	7.989E+00	ns	R424	0 0 0 0 0	

230. C₄H₃BrN₂O₂

5-Bromouracil

5-Bromo-2

4(1H,3H)-Pyrimidinedione

5-Bromo-2,4-dihydroxypyrimidine

Bromouracil

RN: 51-20-7 **MP (°C):** 310
MW: 190.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.507E-02	2.878E+00	25	S471	0 0 0 0 0	
1.908E-02	3.644E+00	25	S471	0 0 0 0 0	
1.350E-02	2.578E+00	25	Z408	0 0 0 0 0	

231. C₄H₃ClN₂O₂

6-Chlorouracil

4-Chloro-2,6-dihydroxypyrimidine

RN: 4270-27-3 **MP (°C):****MW:** 146.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.334E-02	4.885E+00	25	S471	0 0 0 0 0	
3.350E-02	4.909E+00	25	S471	0 0 0 0 0	

232. C₄H₃ClN₂O₂

5-Chlorouracil

RN: 1820-81-1 **MP (°C):****MW:** 146.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.707E-02	2.501E+00	25	S471	0 0 0 0 0	
1.712E-02	2.509E+00	25	S471	0 0 0 0 0	
1.800E-02	2.638E+00	25	Z408	0 0 0 0 0	
9.827E-04	1.440E-01	ns	Y414	0 0 0 0 0	

233. C₄H₃FN₂O₂

5 Fluorouracil

5-Fluorouracil

Fluorouracil

5-Fluoro-2,4(1H,3H)-pyrimidinedione

Fluroblastin

Fluorouracil

RN: 51-21-8 **MP (°C):** 281**MW:** 130.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-02	1.249E+01	21	B416	2 2 1 2 1	
8.533E-02	1.110E+01	22	B321	0 0 0 0 0	pH 4.0
8.533E-02	1.110E+01	22	B332	1 1 0 0 1	pH 4.0
8.533E-02	1.110E+01	22	B388	0 0 0 0 0	
9.379E-02	1.220E+01	22	M317	1 1 1 1 1	
9.379E-02	1.220E+01	25	R023	0 0 0 0 0	
1.356E-01	1.763E+01	25	S471	0 0 0 0 0	
1.382E-01	1.798E+01	25	S471	0 0 0 0 0	
6.940E-02	9.027E+00	25	Z408	0 0 0 0 0	
8.533E-02	1.110E+01	37	B332	0 0 0 0 0	
9.566E-02	1.244E+01	ns	S469	0 0 0 0 0	pH 4.0

234. C₄H₃IN₂O₂

5-Iodouracil

5-Iodo-2,4(1H,3H)-pyrimidinedione

5-Iodo-2,4-dihydroxypyrimidine

RN: 696-07-1 MP (°C): 274–276 (°dec)

MW: 237.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.062E-02	4.907E+00	25	S471	0 0 0 0 0	
2.072E-02	4.931E+00	25	S471	0 0 0 0 0	
1.060E-02	2.523E+00	25	Z408	0 0 0 0 0	

235. C₄H₃N₂S

2-Methyl-1,3,4-thiadiazole

Thiodiazolique methyle

RN: 26584-42-9 MP (°C):

MW: 111.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.918E-03	8.800E-01	37	D084	1 0 1 0 1	

236. C₄H₃N₃O₄

5-Nitrouracil

RN: 611-08-5 MP (°C):

MW: 157.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-02	3.613E+00	25	Z408	0 0 0 0 0	

237. C₄H₃N₃O₅

5-Nitrobarbituric acid

Dilitursaeure

RN: 28176-10-5 MP (°C): 176

MW: 173.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-03	9.000E-01	25.60	F300	1 0 0 0 0	

238. C₄H₄Br₂O₄*meso*-2,3-Dibromosuccinic acid*meso*-Dibrom-bernsteinsaeure

DL-2,3-Dibromosuccinic acid

DL-Dibrom-bernsteinsaeure

RN: 526-78-3 MP (°C): 171

MW: 275.89 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.249E-02	2.000E+01	17	F300	1 0 0 0 2	

239. C₄H₄Cl₂N₂O₂

1,3-Dichloro-5-methylhydantoin

2,4-Imidazolidinedione, 1,3-dichloro-5-methyl-

Hydantoin, 1,3-dichloro-5-methyl-

RN: 15216-12-3 MP (°C):

MW: 182.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.634E-02	2.991E+00	20	B080	1 0 1 1 0	
4.498E-02	8.232E+00	40	B080	1 0 1 1 1	

240. C₄H₄Cl₂O₄

L-2,3-Dichlorosuccinic acid

L(-)-Dichlor-bernsteinsaeure

D-2,3-Dichlorosuccinic acid

D(+)-Dichlor-bernsteinsaeure

2,3-Dichlorosuccinic acid

meso-2,3-Dichlorosuccinic acid

RN: 19922-87-3 MP (°C): 168

MW: 186.98 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.674E+00	5.000E+02	25	H090	0 1 1 1 1	
1.701E-02	3.180E+00	ns	H090	0 2 2 1 2	

241. C₄H₄N₂

Succinonitrile

Bersteinsaeure-dinitril

RN: 110-61-2 MP (°C): 57

MW: 80.09 BP (°C): 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.584E+00	1.269E+02	20	F300	1 0 0 0 2	

242. C₄H₄N₂O

4(3H)-Pyrimidone

4-Hydroxypyrimidine

RN: 51953-17-4 **MP (°C):** 164
MW: 96.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E+00	2.703E+02	20	B050	1 0 0 0 0	

243. C₄H₄N₂O

2-Hydroxypyrimidine

2-Pyrimidinol

RN: 51953-13-0 **MP (°C):**
MW: 96.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.252E+00	3.125E+02	20	B050	1 0 0 0 0	

244. C₄H₄N₂OS

2-Thiouracil

Thiouracil

4(1H)-Pyrimidinone

RN: 141-90-2 **MP (°C):** 340
MW: 128.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.679E-03	5.996E-01	20	D041	1 0 0 0 0	
5.530E-03	7.087E-01	25	G016	1 2 1 2 2	
3.900E-03	4.998E-01	ns	I310	0 0 0 0 0	intrinsic

245. C₄H₄N₂O₂

Uracil

2,4-Dihydroxypyrimidine

RN: 66-22-8 **MP (°C):** 335
MW: 112.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.964E-02	3.322E+00	20	B050	1 0 0 0 0	
2.500E-02	2.802E+00	20	N019	0 0 0 0 0	
3.200E-02	3.587E+00	25	D041	1 0 0 0 1	
3.212E-02	3.600E+00	25	F300	1 0 0 0 1	
2.380E-02	2.668E+00	25	H061	0 0 0 0 0	
4.109E-02	4.605E+00	25	S471	0 0 0 0 0	
4.125E-02	4.624E+00	25	S471	0 0 0 0 0	

(continued)

245. C₄H₄N₂O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-02	3.038E+00	25	Z408	0 0 0 0 0	
4.015E-02	4.500E+00	37	B390	0 0 0 0 0	
2.676E-02	3.000E+00	ns	B177	0 0 0 0 0	

246. C₄H₄N₂O₂

4,6-Dihydroxypyrimidine

4,6-Pyrimidinediol

RN: 1193-24-4 MP (°C): >300

MW: 112.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.225E-02	2.494E+00	20	B050	1 0 0 0 0	

247. C₄H₄N₂O₂

2,4-Dihydroxypyrimidine

RN: 51953-14-1 MP (°C):

MW: 112.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.964E-02	3.322E+00	20	B050	1 0 0 0 0	

248. C₄H₄N₂O₂

Maleic hydrazide

Dihydropyridazine-3,6-dione

RN: 123-33-1 MP (°C):

MW: 112.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.554E-02	3.984E+00	20	B185	0 0 0 0 0	
5.321E-02	5.964E+00	25	B185	0 0 0 0 0	
5.353E-02	6.000E+00	25	B200	1 0 0 0 2	
5.321E-02	5.964E+00	25	M061	1 0 0 0 0	
5.353E-02	6.000E+00	25	M161	1 0 0 0 0	
5.321E-02	5.964E+00	ns	B100	0 0 0 0 0	
6.310E-03	7.072E-01	ns	M163	0 0 0 0 0	EFG
3.554E-02	3.984E+00	ns	N013	0 0 0 0 0	

249. C₄H₄N₂O₃

Barbituric acid

Barbitursaeure

RN: 67-52-7

MP (°C): 248

MW: 128.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-07	1.900E-05	37	B166	1 0 1 1 1	
5.129E-02	6.569E+00	ns	R424	0 0 0 0 0	
5.129E-02	6.569E+00	ns	R427	0 0 0 0 0	

250. C₄H₄N₂O₃

2,4,6-Trihydroxypyrimidine

2,4,6-Pyrimidinetriol

RN: 223674-01-9 MP (°C):

MW: 128.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.170E-02	6.623E+00	20	B050	1 0 0 0 0	

251. C₄H₄O₄*trans*-Fumaric acid

Fumaric acid

Fumarsaeure

RN: 110-17-8 MP (°C): 287

MW: 116.07 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-02	2.295E+00	0	M043	1 0 0 0 1	
3.005E-02	3.488E+00	10	M043	1 0 0 0 1	
4.286E-02	4.975E+00	20	M043	1 0 0 0 1	
5.989E-02	6.951E+00	25	D041	1 0 0 0 1	
6.031E-02	7.000E+00	25	F300	1 0 0 0 0	
5.989E-02	6.951E+00	25	W011	1 2 2 1 1	
6.159E-02	7.149E+00	30	M043	1 0 0 0 1	
9.218E-02	1.070E+01	40	F300	1 0 0 0 2	
9.374E-02	1.088E+01	40	M043	1 0 0 0 1	
9.121E-02	1.059E+01	40	W011	1 2 2 1 2	
1.937E-01	2.248E+01	60	M043	1 0 0 0 1	
2.019E-01	2.344E+01	60	W011	1 2 2 1 1	
4.258E-01	4.943E+01	80	M043	1 0 0 0 1	
7.689E-01	8.925E+01	100	D041	1 0 0 0 1	
8.012E-01	9.300E+01	100	F300	1 0 0 0 1	
7.689E-01	8.925E+01	100	M043	1 0 0 0 1	
7.689E-01	8.925E+01	100	W011	1 2 2 1 1	
5.248E-02	6.092E+00	ns	R424	0 0 0 0 0	

252. C₄H₄O₄

Maleic acid

Maleinsaeure

RN: 110-16-7

MP (°C): 138

MW: 116.07

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.431E+00	2.821E+02	0	M043	1 0 0 0 2	
2.607E+00	3.026E+02	4.99	A339	0 0 0 0 0	
2.872E+00	3.334E+02	10	F300	1 0 0 0 2	
2.872E+00	3.333E+02	10	M043	1 0 0 0 1	
2.880E+00	3.343E+02	9.99	A339	0 0 0 0 0	
3.094E+00	3.591E+02	14.99	A339	0 0 0 0 0	
3.312E+00	3.845E+02	19.99	A339	0 0 0 0 0	
3.547E+00	4.118E+02	20	M043	1 0 0 0 1	
6.789E+00	7.880E+02	22.5	G301	0 0 0 0 0	
3.592E+00	4.170E+02	24.99	A339	0 0 0 0 0	
3.797E+00	4.407E+02	25	D041	1 0 0 0 2	
3.797E+00	4.407E+02	25	F300	1 0 0 0 2	
3.840E+00	4.457E+02	25	H430	0 0 0 0 0	
3.797E+00	4.407E+02	25	W011	1 2 2 1 2	
3.823E+00	4.437E+02	29.99	A339	0 0 0 0 0	
4.081E+00	4.737E+02	30	M043	1 0 0 0 1	
4.117E+00	4.778E+02	34.99	A339	0 0 0 0 0	
4.300E+00	4.991E+02	39.99	A339	0 0 0 0 0	
4.608E+00	5.349E+02	40	M043	1 0 0 0 2	
4.561E+00	5.294E+02	40	W011	1 2 2 1 2	
4.562E+00	5.295E+02	44.99	A339	0 0 0 0 0	
4.677E+00	5.429E+02	49.99	A339	0 0 0 0 0	
4.842E+00	5.620E+02	54.99	A339	0 0 0 0 0	
5.031E+00	5.840E+02	59.99	A339	0 0 0 0 0	
5.516E+00	6.403E+02	60	M043	1 0 0 0 2	
5.151E+00	5.979E+02	60	W011	1 2 2 1 2	
5.166E+00	5.997E+02	64.99	A339	0 0 0 0 0	
6.366E+00	7.389E+02	80	M043	1 0 0 0 2	
6.864E+00	7.967E+02	97.5	D041	1 0 0 0 2	
6.866E+00	7.970E+02	97.5	F300	1 0 0 0 2	
6.866E+00	7.970E+02	97.5	W011	1 2 2 1 2	

253. C₄H₄S

Thiophene

Thiofuran

Thiacyclopentadiene

RN: 110-02-1

MP (°C): -38.3

MW: 84.14

BP (°C): 84.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.583E-02	3.015E+00	25	K119	1 0 0 0 2	
3.583E-02	3.015E+00	25	P051	2 1 1 2 2	
3.583E-02	3.015E+00	25.00	P007	2 1 2 2 2	

254. C₄H₅BrO₄

Bromosuccinic acid

DL-Brombernsteinsaeure

RN: 923-06-8 **MP (°C):**
MW: 196.99 **BP (°C):** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.092E-01	1.200E+02	15.5	F300	1 0 0 0 1	

255. C₄H₅ClO₂

2-Chloroisocrotonic acid

α-Chlor-isocrotonsaeure

RN: 24253-33-6 **MP (°C):**
MW: 120.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.102E-01	6.150E+01	19	F300	1 0 0 0 2	

256. C₄H₅ClO₂

2-Chlorocrotonic acid

α-Chlor-crotonsaeure

RN: 600-13-5 **MP (°C):**
MW: 120.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-01	2.100E+01	19	F300	1 0 0 0 1	

257. C₄H₅ClO₂

3-Chlorocrotonic acid

β-Chlor-crotonsaeure

RN: 6214-28-4 **MP (°C):** 94
MW: 120.54 **BP (°C):** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.842E-01	2.220E+01	12.5	F300	1 0 0 0 2	
2.481E-01	2.990E+01	19	F300	1 0 0 0 2	

258. C₄H₅ClO₂

3-Chloroisocrotonic acid

 β -Chlor-isocrotonsaeure

RN: 6625-00-9 MP (°C):

MW: 120.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.037E-01	1.250E+01	7	F300	1 0 0 0 2	
1.560E-01	1.880E+01	19	F300	1 0 0 0 2	

259. C₄H₅ClO₄

L-Chlorosuccinic acid

L(-)-Chlor-bernsteinsaeure

D-Chlorosuccinic acid

D(+)-Chlor-bernsteinsaeure

RN: 16045-92-4 MP (°C):

MW: 152.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E+00	1.800E+02	20	F300	1 0 0 0 1	
1.193E+00	1.820E+02	20	F300	1 0 0 0 2	

260. C₄H₅F₃O

Fluroxene

2,2,2-(Trifluoroethoxy)ethene

Redeptin

Fluoromar

RN: 406-90-6 MP (°C):

MW: 126.08 BP (°C): 42.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.173E-05	4.000E-03	ns	R028	0 0 0 0 0	

261. C₄H₅N

Pyrrole

Azole

Imidole

RN: 109-97-7 MP (°C): -23

MW: 67.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.098E-01	4.762E+01	rt	B099	0 2 0 0 0	

262. C₄H₅N

Methacrylonitrile

2-Methyl-2-propenenitrile

RN: 126-98-7 **MP (°C):** -35.8
MW: 67.09 **BP (°C):** 90.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.692E-01	2.477E+01	25	L096	1 2 0 2 2	

263. C₄H₅NO₂

Hymexazol

3-Hydroxy-5-methyl isoxazole

5-Methyl-3(2H)-isoxazolone

Tachigaren

Isoxazolol, 5-methyl-

RN: 10004-44-1 **MP (°C):** 86
MW: 99.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.578E-01	8.500E+01	25	M161	1 0 0 0 2	
8.578E-01	8.500E+01	25	N306	1 0 0 0 1	

264. C₄H₅NO₂

Succinimide

2,5-Pyrrolidinedione

Butanimide

RN: 123-56-8 **MP (°C):** 126
MW: 99.09 **BP (°C):** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.174E-01	9.091E+01	0	M043	1 0 0 0 1	
1.392E+00	1.379E+02	10	M043	1 0 0 0 1	
2.082E+00	2.063E+02	20	M043	1 0 0 0 1	
1.978E+00	1.960E+02	21	F300	1 0 0 0 2	
3.273E+00	3.243E+02	30	M043	1 0 0 0 1	
4.577E+00	4.536E+02	40	M043	1 0 0 0 1	
5.887E+00	5.833E+02	60	M043	1 0 0 0 2	
6.868E+00	6.805E+02	80	M043	1 0 0 0 2	
1.413E+00	1.400E+02	ns	D072	0 0 0 0 1	
1.995E+00	1.977E+02	ns	R424	0 0 0 0 0	

265. C₄H₅NS

Allyl isothiocyanate

Allyl mustardol

Allylsenfoel

RN: 57-06-7

MP (°C): -8

MW: 99.16

BP (°C): 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.017E-02	2.000E+00	20	F300	1 0 0 0 0	

266. C₄H₅N₃O

Cytosine

2-Oxy-4-amino pyrimidine

2(1H)-Pyrimidinone, 4-amino-

RN: 71-30-7

MP (°C): 320

MW: 111.10

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	5.555E+00	20	C017	2 0 0 1 0	EFG
6.877E-02	7.641E+00	25	D041	1 0 0 0 1	
7.200E-02	8.000E+00	25	F300	1 0 0 0 0	
6.580E-02	7.311E+00	25	H061	0 0 0 0 0	
6.500E-02	7.222E+00	25	R030	0 0 0 0 0	

267. C₄H₅N₃OS

6-Amino-2-thiouracil

2-Mercapto-4-amino-6-hydroxypyrimidine

2-Thio-4-amino-6-hydroxypyrimidine

2-Mercapto-6-aminouracil

RN: 1004-40-6

MP (°C):

MW: 143.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.790E-03	2.563E-01	25	G016	1 2 1 2 2	intrinsic

268. C₄H₅N₃O₂

5-Aminouracil

5-Amino-uracil

RN: 932-52-5

MP (°C): >300

MW: 127.10

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.934E-03	5.000E-01	20	F300	1 0 0 0 0	
4.700E-03	5.974E-01	25	Z408	0 0 0 0 0	
1.259E-01	1.600E+01	100	F300	1 0 0 0 1	

269. C₄H₅N₃O₂

6-Aminouracil

2,4(1H,3H)-Pyrimidinedione, 6-amino

4-Amino-2,6-dihydroxypyrimidine

6-Amino-2,4-pyrimidinediol

4-Amino uracil

RN: 873-83-6 **MP (°C):****MW:** 127.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-03	5.974E-01	25	Z408	0 0 0 0 0	

270. C₄H₅N₃O₂

2-Methyl-4(5)-nitroimidazole

2-Methyl-5-nitroimidazole

Menidazole

RP 8532

L 581490

RN: 696-23-1 **MP (°C):** 257–258**MW:** 127.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.368E-02	3.010E+00	20	D344	0 0 0 0 0	
2.367E-02	3.009E+00	20	D344	0 0 0 0 0	
2.353E-02	2.991E+00	20	D344	0 0 0 0 0	
2.370E-02	3.012E+00	20	D344	0 0 0 0 0	

271. C₄H₆

1,3-Butadiene

Pyrrolylene

RN: 106-99-0 **MP (°C):** -108.9**MW:** 54.09 **BP (°C):** -4.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.359E-02	7.350E-01	25	M001	2 1 2 2 2	

272. C₄H₆

1-Butyne

Ethylacetylene

Ethylethyne

RN: 107-00-6 **MP (°C):** -125.7**MW:** 54.09 **BP (°C):** 8.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.306E-02	2.870E+00	25	M001	2 1 2 2 2	

273. C₄H₆BrNO₄

5-Bromo-5-nitro-1,3-dioxane

Bronidox

Microcide I

Bronidox L

1,3-Dioxane, 5-bromo-5-nitro-

RN: 30007-47-7 **MP (°C):** 49–50**MW:** 212.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.706E-02	5.737E+00	25	L013	1 0 2 1 2	

274. C₄H₆Cl₂O₂S

3,4-Dichlorotetrahydrothiophene dioxide

3,4-Dichlorotetrahydrothiophene 1,1-dioxide

3,4-Dichlorosulfolane

DAC PRD

3,4-Dichlorothiolane 1,1-dioxide

RN: 3001-57-8 **MP (°C):** 130**MW:** 189.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.161E-02	2.195E+00	20	M061	1 0 0 0 1	

275. C₄H₆N₂O₂

2,5-Piperazinedione

Diketopiperazine

RN: 106-57-0 **MP (°C):****MW:** 114.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.232E-01	1.406E+01	20	B032	1 2 2 1 2	
1.253E-01	1.430E+01	20	M075	2 0 1 1 2	
1.475E-01	1.683E+01	25	B032	1 2 2 1 2	
1.754E-01	2.001E+01	29.80	B032	1 2 2 1 2	

276. C₄H₆N₂S₄Zn

Zineb

Zinc ethylenebis(dithiocarbamate)

RN: 12122-67-7 **MP (°C):****MW:** 275.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.627E-06	1.000E-03	20	M061	1 0 0 0 0	
3.627E-05	1.000E-02	rt	M161	0 0 0 0 1	

277. C₄H₆N₄O₃

Allantoin

Allantoine

RN: 97-59-6

MP (°C): 238

MW: 158.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.303E-02	5.223E+00	20	D041	1 0 0 0 2	
4.755E-02	7.519E+00	c	D004	0 0 0 0 0	
2.040E-01	3.226E+01	h	D004	0 0 0 0 0	
2.530E-02	4.000E+00	ns	D072	0 0 0 0 1	

278. C₄H₆N₄O₃S₂

Acetazolamide

5-Acetamido-1,3,4-thiadiazole-2-sulfonamide

RN: 59-66-5

MP (°C): 258

MW: 222.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-03	6.001E-01	15	K024	1 2 1 1 2	
2.249E-03	4.998E-01	20	D041	1 0 0 0 0	
3.200E-03	7.112E-01	25	C415	1 0 0 1 0	
2.216E-03	4.925E-01	25	F415	0 0 0 0 0	Average
4.409E-03	9.799E-01	30	E049	2 0 2 2 2	
5.174E-03	1.150E+00	37	C054	2 0 2 1 2	
2.880E-03	6.400E-01	amb	L434	0 0 0 0 0	
>2.25E-03	>5.00E-01	ns	B404	0 2 1 1 0	
4.144E-03	9.210E-01	ns	I304	0 0 0 0 0	
4.500E-04	1.000E-01	ns	K444	0 0 0 0 0	
4.365E-03	9.701E-01	ns	R428	0 0 0 0 0	

279. C₄H₆O

Vinyl ether

1,1'-Oxybisethene

Divinyl ether

RN: 109-93-3

MP (°C):

MW: 70.09

BP (°C): 28.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.490E-02	5.250E+00	37	R047	0 0 0 0 0	
5.487E-01	3.846E+01	ns	R028	0 0 0 0 0	

280. C₄H₆O

Crotonaldehyde

But-*trans*-enal

RN: 4170-30-3

MP (°C): -76.5

MW: 70.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+2.14E+00	+1.50E+02	ns	S460	0 0 0 0 0	

281. C₄H₆O

α-Methylacrolein

α-Methyl-acrolein

RN: 78-85-3

MP (°C):

MW: 70.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.089E-01	5.670E+01	20	F300	1 0 0 0 2	
1.236E+00	8.663E+01	ns	S460	0 0 0 0 0	

282. C₄H₆O*trans*-Crotonaldehyde

Crotonaldehyd

RN: 123-73-9

MP (°C): -77

MW: 70.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.140E+00	1.500E+02	20	F300	1 0 0 0 1	

283. C₄H₆O₂

Diacetyl

2,3-Butanedione

RN: 431-03-8

MP (°C):

MW: 86.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E+00	2.000E+02	15	F300	1 0 0 0 1	
2.323E+00	2.000E+02	20	D041	1 0 0 0 1	

284. C₄H₆O₂

Methyl acrylate

Acrylic acid methyl ester

2-Propenoic acid methyl ester

RN: 96-33-3

MP (°C): -76.5

MW: 86.09

BP (°C): 70

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.742E-01	4.943E+01	30	L096	1 2 0 2 1	

285. C₄H₆O₂*trans*-Crotonic acid*trans*-Crotonsaeure

RN: 3724-65-0

MP (°C):

MW: 86.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.989E-01	8.600E+01	25	F300	1 0 0 0 1	
4.600E+00	3.960E+02	40	F300	1 0 0 0 2	

286. C₄H₆O₂

Vinyl acetate

Vinylacetate

RN: 108-05-4

MP (°C): -100

MW: 86.09

BP (°C): 72

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.136E-01	2.700E+01	50	L097	1 1 1 1 1	

287. C₄H₆O₂

Crotonic acid

2-Butenoic acid

3-Methylacrylic acid

RN: 107-93-7

MP (°C): 73

MW: 86.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.882E-01	7.647E+01	20	D041	1 0 0 0 2	

288. C₄H₆O₂ α -Butyrolactone3-Hydroxybutanoic acid β -lactone

RN: 3068-88-0

MP (°C):

MW: 86.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.541E+00	1.327E+02	18	I313	0 0 0 0 0	

289. C₄H₆O₂S₄

bis(Methylxanthogen) disulfide

Dimethylxanthogen disulfide

Methyl dixanthogen

RN: 1468-37-7 MP (°C): 22.75

MW: 214.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-04	2.465E-02	25	H102	1 2 1 2 2	

290. C₄H₆O₃

Acetic anhydride

Essigsaeure-anhydrid

RN: 108-24-7 MP (°C): -73

MW: 102.09 BP (°C): 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E+00	1.200E+02	20	F300	1 0 0 0 2	

291. C₄H₆O₄

Methylmalonic acid

Acide methylmalonique

Methyl-malonsaeure

RN: 516-05-2 MP (°C): 129.5

MW: 118.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E+00	3.070E+02	0	F300	1 0 0 0 2	
3.743E+00	4.420E+02	0	M051	1 0 0 0 2	
4.954E+00	5.850E+02	15	M051	1 0 0 0 2	
5.750E+00	6.790E+02	25	M051	1 0 0 0 2	
4.071E+00	4.808E+02	50	F300	1 0 0 0 2	
7.748E+00	9.150E+02	50	M051	1 0 0 0 2	

292. C₄H₆O₄

Succinic acid

Bernsteinsaeure

RN: 110-15-6 MP (°C): 185

MW: 118.09 BP (°C): 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.363E-01	2.790E+01	0	L041	1 0 0 1 2	
2.273E-01	2.684E+01	0	M020	1 0 0 1 1	
2.306E-01	2.724E+01	0	M043	1 0 0 0 1	

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292. C₄H₆O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.892E-01	3.415E+01	4.99	A339	0 0 0 0 0	
3.569E-01	4.215E+01	10	M043	1 0 0 0 1	
3.616E-01	4.271E+01	9.99	A339	0 0 0 0 0	
3.854E-01	4.551E+01	11.85	L064	2 2 2 1 2	
4.518E-01	5.335E+01	14.99	A339	0 0 0 0 0	
4.102E-01	4.843E+01	15	F055	1 2 2 2 2	
4.149E-01	4.900E+01	15	L041	1 0 0 1 1	
4.149E-01	4.900E+01	15	M051	1 0 0 0 1	
4.912E-01	5.800E+01	17.50	F300	1 0 0 0 1	
4.974E-01	5.874E+01	18	L064	2 2 2 1 2	
5.661E-01	6.685E+01	19.99	A339	0 0 0 0 0	
5.392E-01	6.367E+01	20	D041	1 0 0 0 1	
5.019E-01	5.927E+01	20	F055	1 2 2 2 2	
5.420E-01	6.400E+01	20	F300	1 0 0 0 2	
4.912E-01	5.800E+01	20	L041	1 0 0 1 1	
5.466E-01	6.455E+01	20	M043	1 0 0 0 1	
5.510E-01	6.507E+01	20	M153	1 0 0 0 0	cal. from fitted equation
4.632E-01	5.470E+01	20	M171	1 0 0 0 1	
5.716E-01	6.750E+01	20	W026	1 0 1 1 1	average of 2
6.344E-01	7.492E+01	23.75	L064	2 2 2 1 2	
6.829E-01	8.064E+01	24.99	A339	0 0 0 0 0	
5.930E-01	7.003E+01	25	D061	1 0 0 0 2	
6.032E-01	7.124E+01	25	F055	1 2 2 2 2	
6.849E-01	8.088E+01	25	H430	0 0 0 0 0	
6.518E-01	7.697E+01	25	M020	1 0 0 1 2	
6.634E-01	7.834E+01	25	M153	1 0 0 0 0	cal. from fitted equation
7.402E-01	8.741E+01	28	D050	1 2 1 2 2	
8.003E-01	9.451E+01	29.99	A339	0 0 0 0 0	
8.047E-01	9.502E+01	30	M043	1 0 0 0 2	
8.047E-01	9.502E+01	30	M153	1 0 0 0 0	cal. from fitted equation
8.849E-01	1.045E+02	30	W026	1 0 1 1 2	average of 2
9.508E-01	1.123E+02	34.99	A339	0 0 0 0 0	
8.976E-01	1.060E+02	35	L041	1 0 0 1 2	
9.742E-01	1.150E+02	35	M153	1 0 0 0 0	cal. from fitted equation
1.145E+00	1.353E+02	39.99	A339	0 0 0 0 0	
1.149E+00	1.357E+02	40	B088	1 0 0 0 2	
1.181E+00	1.394E+02	40	M043	1 0 0 0 2	
1.168E+00	1.379E+02	40	M153	1 0 0 0 0	cal. from fitted equation
1.377E+00	1.627E+02	44.99	A339	0 0 0 0 0	
1.600E+00	1.889E+02	49.99	A339	0 0 0 0 0	
1.524E+00	1.800E+02	50	L041	1 0 0 1 2	
1.633E+00	1.929E+02	50	M020	1 0 0 1 2	
1.842E+00	2.175E+02	54.99	A339	0 0 0 0 0	
2.048E+00	2.418E+02	59.99	A339	0 0 0 0 0	
2.232E+00	2.636E+02	60	M043	1 0 0 0 2	
2.398E+00	2.832E+02	64.99	A339	0 0 0 0 0	
2.380E+00	2.810E+02	65	L041	1 0 0 1 2	
3.238E+00	3.824E+02	75	F300	1 0 0 0 2	
3.191E+00	3.768E+02	75	M020	1 0 0 1 2	

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292. C₄H₆O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E+00	4.145E+02	80	M043	1 0 0 0 2	
8.515E-01	1.006E+02	84.30	B118	1 0 0 0 2	unit assumed
4.636E+00	5.475E+02	100	D041	1 0 0 0 2	
4.738E+00	5.595E+02	100	M043	1 0 0 0 2	
6.821E-01	8.054E+01	rt	H431	0 0 0 0 0	

293. C₄H₆O₄

Methyl oxalate

Oxalic acid ethyl ester

Oxalsaeure-monoaethyl ester

RN: 553-90-2 MP (°C): 54.0
 MW: 118.09 BP (°C): 163.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
3.006E-01	3.549E+01	.1	K079	1 0 0 0 2	
6.900E-01	8.148E+01	11.1	K079	1 0 0 0 2	
1.029E+00	1.216E+02	19.5	K079	1 0 0 0 2	
5.106E-01	6.030E+01	25	F300	1 0 0 0 2	
1.489E+00	1.758E+02	27.1	K079	1 0 0 0 2	
1.867E+00	2.204E+02	31.9	K079	1 0 0 0 2	
2.978E+00	3.516E+02	44.4	K079	1 0 0 0 2	
3.372E+00	3.982E+02	49.2	K079	1 0 0 0 2	
3.589E+00	4.238E+02	51.0	K079	1 0 0 0 2	
3.839E+00	4.533E+02	53.0	K079	1 0 0 0 2	
4.783E+00	5.649E+02	75.0	K079	1 0 0 0 2	
4.939E+00	5.832E+02	79.3	K079	1 0 0 0 2	
5.678E+00	6.705E+02	96.1	K079	1 0 0 0 2	
4.929E-01	5.820E+01	rt	D021	0 0 1 1 2	

294. C₄H₆O₅

D-Malic acid

D(-)-Aepfelsaeure

RN: 636-61-3 MP (°C): 100
 MW: 134.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
3.397E+00	4.555E+02	4.99	A339	0 0 0 0 0	
3.542E+00	4.749E+02	9.99	A339	0 0 0 0 0	
3.695E+00	4.954E+02	14.99	A339	0 0 0 0 0	
3.878E+00	5.200E+02	19.99	A339	0 0 0 0 0	
4.030E+00	5.403E+02	24.99	A339	0 0 0 0 0	
4.146E+00	5.560E+02	29.99	A339	0 0 0 0 0	
4.282E+00	5.742E+02	34.99	A339	0 0 0 0 0	
4.441E+00	5.955E+02	39.99	A339	0 0 0 0 0	
4.544E+00	6.094E+02	44.99	A339	0 0 0 0 0	

(continued)

294. C₄H₆O₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.719E+00	6.328E+02	49.99	A339	0 0 0 0 0	
4.840E+00	6.490E+02	54.99	A339	0 0 0 0 0	
4.976E+00	6.672E+02	59.99	A339	0 0 0 0 0	
5.119E+00	6.865E+02	64.99	A339	0 0 0 0 0	

295. C₄H₆O₅

Diglycolic acid

Di-glykolsaeure

RN: 110-99-6

MP (°C): 148

MW: 134.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E+00	2.140E+02	5.09	A340	0 0 0 0 0	
1.932E+00	2.590E+02	10.99	A340	0 0 0 0 0	
2.522E+00	3.382E+02	15.59	A340	0 0 0 0 0	
2.668E+00	3.577E+02	20.59	A340	0 0 0 0 0	
2.834E+00	3.801E+02	23.49	A340	0 0 0 0 0	
3.252E+00	4.361E+02	28.09	A340	0 0 0 0 0	
3.645E+00	4.887E+02	37.49	A340	0 0 0 0 0	
3.794E+00	5.087E+02	39.99	A340	0 0 0 0 0	
4.061E+00	5.445E+02	47.99	A340	0 0 0 0 0	
4.135E+00	5.545E+02	49.99	A340	0 0 0 0 0	
4.353E+00	5.837E+02	54.49	A340	0 0 0 0 0	
4.508E+00	6.044E+02	59.49	A340	0 0 0 0 0	
4.631E+00	6.209E+02	64.99	A340	0 0 0 0 0	
4.776E+00	6.404E+02	69.99	A340	0 0 0 0 0	
4.877E+00	6.540E+02	74.99	A340	0 0 0 0 0	
4.969E+00	6.663E+02	79.89	A340	0 0 0 0 0	
5.067E+00	6.794E+02	83.99	A340	0 0 0 0 0	
5.125E+00	6.872E+02	88.19	A340	0 0 0 0 0	

296. C₄H₆O₅

DL-Malic acid

Malic acid

RN: 6915-15-7

MP (°C): 131.5

MW: 134.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.512E+00	4.709E+02	0	M043	1 0 0 0 1	
3.820E+00	5.122E+02	10	M043	1 0 0 0 2	
4.158E+00	5.575E+02	20	M043	1 0 0 0 2	
4.414E+00	5.918E+02	25	H430	0 0 0 0 0	
4.401E+00	5.902E+02	26	D041	1 0 0 0 2	
4.415E+00	5.920E+02	26	F300	1 0 0 0 2	

(continued)

296. C₄H₆O₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.605E+00	7.516E+02	30	D062	1 0 1 1 0	data given in normality
4.475E+00	6.000E+02	30	M043	1 0 0 0 2	
4.794E+00	6.429E+02	40	M043	1 0 0 0 2	
5.442E+00	7.297E+02	60	M043	1 0 0 0 2	
5.998E+00	8.043E+02	79	D041	1 0 0 0 2	
6.033E+00	8.089E+02	79	F300	1 0 0 0 2	
6.126E+00	8.214E+02	80	M043	1 0 0 0 2	

297. C₄H₆O₆*meso*-Tartaric acid*meso*-Weinsaeure

RN: 147-73-9

MP (°C): 147

MW: 150.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E+00	3.360E+02	0	F300	1 0 0 0 2	
3.702E+00	5.556E+02	15	D041	1 0 0 0 2	
3.731E+00	5.600E+02	15	F300	1 0 0 0 1	
3.731E+00	5.600E+02	20	F300	1 0 0 0 1	

298. C₄H₆O₆D-(*–*)Tartaric acidD-(*–*)-Dihydroxysuccinic acid

RN: 147-71-7

MP (°C): 173

MW: 150.09

BP (°C): 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.564E+00	5.349E+02	0	M043	1 0 0 0 2	
3.348E+00	5.024E+02	4.99	A339	0 0 0 0 0	
2.350E+00	3.528E+02	10	D020	1 2 1 1 2	
3.715E+00	5.575E+02	10	M043	1 0 0 0 2	
3.431E+00	5.149E+02	9.99	A339	0 0 0 0 0	
3.499E+00	5.251E+02	14.99	A339	0 0 0 0 0	
3.553E+00	5.332E+02	19.99	A339	0 0 0 0 0	
3.875E+00	5.816E+02	20	M043	1 0 0 0 2	
3.629E+00	5.447E+02	24.99	A339	0 0 0 0 0	
2.459E+00	3.691E+02	25	D020	1 2 1 1 2	
3.973E+00	5.963E+02	25	F017	1 0 0 0 2	
3.706E+00	5.562E+02	29.99	A339	0 0 0 0 0	
4.060E+00	6.094E+02	30	M043	1 0 0 0 2	
3.791E+00	5.690E+02	34.99	A339	0 0 0 0 0	
3.846E+00	5.773E+02	39.99	A339	0 0 0 0 0	
4.249E+00	6.377E+02	40	M043	1 0 0 0 2	
3.926E+00	5.892E+02	44.99	A339	0 0 0 0 0	

(continued)

298. C₄H₆O₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.021E+00	6.036E+02	49.99	A339	0 0 0 0 0	
4.104E+00	6.160E+02	54.99	A339	0 0 0 0 0	
4.157E+00	6.238E+02	59.99	A339	0 0 0 0 0	
4.581E+00	6.875E+02	60	M043	1 0 0 0 2	
4.232E+00	6.352E+02	64.99	A339	0 0 0 0 0	
4.876E+00	7.319E+02	80	M043	1 0 0 0 2	
5.159E+00	7.743E+02	100	M043	1 0 0 0 2	

299. C₄H₆O₆

L-Tartaric acid

L(+)-Weinsaeure

L(+)-Tartaric acid

RN: 87-69-4

MP (°C): 169

MW: 150.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.565E+00	5.350E+02	0	F300	1 0 0 0 2	
3.564E+00	5.349E+02	0	F302	1 0 0 0 2	
3.634E+00	5.455E+02	5	F302	1 0 0 0 2	
3.702E+00	5.556E+02	10	F302	1 0 0 0 2	
3.791E+00	5.690E+02	15	F302	1 0 0 0 2	
3.878E+00	5.820E+02	20	F300	1 0 0 0 2	
3.875E+00	5.816E+02	20	F302	1 0 0 0 2	
3.965E+00	5.951E+02	25	F302	1 0 0 0 2	
4.060E+00	6.094E+02	30	F302	1 0 0 0 2	
4.158E+00	6.241E+02	35	F302	1 0 0 0 2	
4.249E+00	6.377E+02	40	F302	1 0 0 0 2	
4.325E+00	6.491E+02	45	F302	1 0 0 0 2	
4.397E+00	6.600E+02	50	F300	1 0 0 0 1	
4.404E+00	6.610E+02	50	F302	1 0 0 0 2	
4.485E+00	6.732E+02	55	F302	1 0 0 0 2	
4.568E+00	6.855E+02	60	F302	1 0 0 0 2	
4.644E+00	6.970E+02	65	F302	1 0 0 0 2	
4.726E+00	7.093E+02	70	F302	1 0 0 0 2	
4.802E+00	7.207E+02	75	F302	1 0 0 0 2	
4.876E+00	7.319E+02	80	F302	1 0 0 0 2	
4.954E+00	7.436E+02	85	F302	1 0 0 0 2	
5.026E+00	7.543E+02	90	F302	1 0 0 0 2	
5.095E+00	7.647E+02	95	F302	1 0 0 0 2	
5.157E+00	7.740E+02	100	F300	1 0 0 0 2	
5.159E+00	7.743E+02	100	F302	1 0 0 0 2	

300. C₄H₆O₆

DL-Tartaric acid

DL-Weinsaeure

Tartaric acid (racemic)

RN: 133-37-9**MP (°C):** 206**MW:** 150.09**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.279E+00	3.421E+02	0	D039	2 2 1 2 0	EFG
5.630E-01	8.450E+01	0	D041	1 0 0 0 2	
5.084E-01	7.630E+01	0	F300	1 0 0 0 2	
5.049E-01	7.579E+01	0	M043	1 0 0 0 1	
2.333E+00	3.502E+02	10	D039	2 2 1 2 0	EFG
7.298E-01	1.095E+02	10	M043	1 0 0 0 2	
2.350E+00	3.528E+02	20	D039	2 2 1 2 0	EFG
1.138E+00	1.708E+02	20	D041	1 0 0 0 2	
1.139E+00	1.710E+02	20	F300	1 0 0 0 2	
1.016E+00	1.525E+02	20	M043	1 0 0 0 2	
2.459E+00	3.690E+02	25	D039	2 2 1 2 2	EFG
1.179E+00	1.770E+02	25	F017	1 0 0 0 2	
1.026E+01	1.540E+03	25	K040	1 0 2 1 2	
2.483E+00	3.726E+02	30	D039	2 2 1 2 0	EFG
1.341E+00	2.013E+02	30	M043	1 0 0 0 2	
2.563E+00	3.846E+02	40	D039	2 2 1 2 0	EFG
1.799E+00	2.701E+02	40	M043	1 0 0 0 2	
2.612E+00	3.921E+02	50	D039	2 2 1 2 0	EFG
2.687E+00	4.033E+02	60	D039	2 2 1 2 0	EFG
2.612E+00	3.921E+02	60	M043	1 0 0 0 2	
2.750E+00	4.128E+02	70	D039	2 2 1 2 0	EFG
2.811E+00	4.220E+02	80	D039	2 2 1 2 0	EFG
3.299E+00	4.952E+02	80	M043	1 0 0 0 2	
2.860E+00	4.292E+02	90	D039	2 2 1 2 0	EFG
2.920E+00	4.382E+02	100	D039	2 2 1 2 0	EFG
4.324E+00	6.490E+02	100	D041	1 0 0 0 2	
4.331E+00	6.500E+02	100	F300	1 0 0 0 1	
3.863E+00	5.798E+02	100	M043	1 0 0 0 2	

301. C₄H₇Br

4-Bromo-1-butene

1-Bromo-3-butene

Homoallyl bromide

4-Bromobutene-1

3-Butenyl bromide

RN: 5162-44-7**MP (°C):****MW:** 135.01**BP (°C):** 98.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.660E-03	7.642E-01	25	M342	1 0 1 1 2	

302. C₄H₇BrN₂O₂Propanamide, *N*-(aminocarbonyl)-2-bromo-

(2-Bromopropionyl)urea

 α -Bromopropionylurea**RN:** 14299-55-9 **MP (°C):****MW:** 195.02 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.581E-01	5.033E+01	ns	F056	0 2 2 2 1	

303. C₄H₇BrO₂ α -Bromobutyric acid

DL-2-Bromobutyric acid

DL-Brombuttersaeure

RN: 80-58-0 **MP (°C):** -4**MW:** 167.01 **BP (°C):** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.191E-01	7.000E+01	ns	F300	1 0 0 0 0	

304. C₄H₇Cl

1-Chloro-2-butene

1-Chloro-2-methylpropene-2

 α -Methylallyl chloride**RN:** 591-97-9 **MP (°C):****MW:** 90.55 **BP (°C):** 84

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E-02	9.990E-01	ns	M061	0 0 0 0 0	

305. C₄H₇Cl₂O₄P

Dichlorvos

O,O-Dimethyl *O*-2-dichlorovinyl phosphate**RN:** 62-73-7 **MP (°C):****MW:** 220.98 **BP (°C):** 84

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.481E-02	9.901E+00	ns	M061	0 0 0 0 0	
4.525E-02	1.000E+01	rt	M161	0 0 0 0 1	

306. C₄H₇Cl₃O1,1,1-Trichloro-*tert*-butanol

Acetonchloroform

Chloretton

RN: 57-15-8**MP (°C):** 98**MW:** 177.46**BP (°C):** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.508E-02	8.000E+00	20	F300	1 0 0 0 0	
4.467E-02	7.927E+00	ns	R424	0 0 0 0 0	
4.467E-02	7.927E+00	ns	R427	0 0 0 0 0	

307. C₄H₇N*n*-Butyronitrile γ -Butyronitrile

Propyl cyanide

1-Cyanopropane

n-Butyronitrile**RN:** 109-74-0**MP (°C):** -112**MW:** 69.11**BP (°C):** 115–117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.446E-02	3.764E+00	25	B004	0 0 0 0 0	

308. C₄H₇NO₂S

4-Thiazolidinecarboxylic acid

Thiazolidine-4-carboxylic acid

 γ -Thiaproline

4-Carboxythiazolidine

Detoxepa

Thiaproline

RN: 444-27-9**MP (°C):** 196–201**MW:** 133.17**BP (°C):** 350.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-01	2.930E+01	21	B414	1 0 0 1 1	

309. C₄H₇NO₃

N-Acetyl glycine

Aceturic acid

Glycin-N-acetat

Glycine-N-acetate

RN: 543-24-8

MP (°C): 206

MW: 117.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.246E-01	2.630E+01	15	F300	1 0 0 0 2	

310. C₄H₇NO₄

Butanoic acid, 4-amino-2-hydroxy-4-oxo-

D-β-Malaminsaeure

L-β-Malaminsaeure

RN: 82310-91-6

MP (°C): 149

MW: 133.10

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.903E-01	3.865E+01	18	L039	1 0 0 0 2	
5.255E-01	6.994E+01	18	L039	1 0 0 0 2	

311. C₄H₇NO₄

DL-Aspartic acid

DL-2-Aminobutanedioic acid

RN: 617-45-8

MP (°C):

MW: 133.10

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.367E-02	3.151E+00	0	D018	2 2 2 1 2	
2.420E-02	3.221E+00	4.99	A405	2 0 1 1 2	
3.140E-02	4.179E+00	9.99	A405	2 0 1 1 2	
3.910E-02	5.204E+00	14.99	A405	2 0 1 1 2	
4.850E-02	6.456E+00	19.99	A405	2 0 1 1 2	
5.900E-02	7.853E+00	24.99	A405	2 0 1 1 2	
6.081E-02	8.094E+00	25	D018	2 2 2 1 2	
6.110E-02	8.133E+00	25	D041	1 0 0 0 1	
7.260E-02	9.663E+00	29.99	A405	2 0 1 1 2	
8.770E-02	1.167E+01	33.99	A405	2 0 1 1 2	
8.950E-02	1.191E+01	34.99	A405	2 0 1 1 2	
1.069E-01	1.423E+01	38.99	A405	2 0 1 1 2	
1.109E-01	1.476E+01	39.99	A405	2 0 1 1 2	
1.293E-01	1.721E+01	44.99	A405	2 0 1 1 2	
1.561E-01	2.078E+01	49.49	A405	2 0 1 1 2	
1.544E-01	2.055E+01	50	D018	2 2 2 1 2	
1.812E-01	2.412E+01	54.99	A405	2 0 1 1 2	
2.170E-01	2.888E+01	58.99	A405	2 0 1 1 2	

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311. C₄H₇NO₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.543E-01	3.385E+01	61.99	A405	2 0 1 1 2	
3.101E-01	4.128E+01	65.99	A405	2 0 1 1 2	
3.284E-01	4.371E+01	68.99	A405	2 0 1 1 2	
3.646E-01	4.853E+01	70.99	A405	2 0 1 1 2	
3.437E-01	4.575E+01	75	D018	2 2 2 1 2	
3.434E-01	4.571E+01	75	D041	1 0 0 0 2	

312. C₄H₇NO₄

Iminodiacetic acid

Imino-diessigsaeure

RN: 142-73-4 MP (°C): 247.5

MW: 133.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.781E-01	2.370E+01	5	F300	1 0 0 0 2	

313. C₄H₇NO₄

L-Aspartic acid

Aspartic acid

L(+)-Asparaginsaeure

L-(+)-Asparagine acid

L-(+)-Aspartic acid

RN: 56-84-8 MP (°C): 270.5

MW: 133.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-02	2.230E+00	0	D018	2 2 2 1 2	
1.780E-02	2.369E+00	4.99	A405	2 0 1 1 2	
2.170E-02	2.888E+00	9.99	A405	2 0 1 1 2	
2.570E-02	3.421E+00	14.99	A405	2 0 1 1 2	
3.160E-02	4.206E+00	19.99	A405	2 0 1 1 2	
3.170E-02	4.220E+00	20	B032	1 2 2 1 2	
3.750E-02	4.991E+00	24.99	A405	2 0 1 1 2	
3.770E-02	5.018E+00	25	B032	1 2 2 1 2	
4.030E-02	5.364E+00	25	D018	2 2 2 1 2	
3.738E-02	4.975E+00	25	D041	1 0 0 0 0	
3.805E-02	5.064E+00	25	G315	0 0 0 0 0	
3.719E-02	4.950E+00	25	J303	0 0 0 0 0	
3.644E-02	4.850E+00	27	D036	0 0 0 0 0	
4.469E-02	5.948E+00	29.80	B032	1 2 2 1 2	
4.550E-02	6.056E+00	29.99	A405	2 0 1 1 2	
5.320E-02	7.081E+00	33.99	A405	2 0 1 1 2	
6.520E-02	8.678E+00	39.99	A405	2 0 1 1 2	
6.348E-02	8.450E+00	40	J303	0 0 0 0 0	

(continued)

313. C₄H₇NO₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.610E-02	1.013E+01	44.99	A405	2 0 1 1 2	
9.304E-02	1.238E+01	50	D018	2 2 2 1 2	
9.110E-02	1.213E+01	50.99	A405	2 0 1 1 2	
1.013E-01	1.348E+01	54.99	A405	2 0 1 1 2	
1.216E-01	1.619E+01	59.99	A405	2 0 1 1 2	
1.232E-01	1.640E+01	60	J303	0 0 0 0 0	
1.316E-01	1.752E+01	62.99	A405	2 0 1 1 2	
1.440E-01	1.917E+01	64.99	A405	2 0 1 1 2	
1.498E-01	1.994E+01	66.99	A405	2 0 1 1 2	
1.725E-01	2.296E+01	69.99	A405	2 0 1 1 2	
1.985E-01	2.642E+01	75	D018	2 2 2 1 2	
2.100E-01	2.795E+01	75	D041	1 0 0 0 2	
2.885E-01	3.840E+01	99	M160	2 1 1 1 0	
3.750E-02	4.991E+00	ns	M025	0 2 0 1 2	
3.738E-02	4.975E+00	rt	H431	0 0 0 0 0	

314. C₄H₇NO₄

L-β-Malamidic acid

L-β-Malaminsaeure

RN: 57229-74-0 MP (°C): 149
 MW: 133.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.242E-01	6.977E+01	18	L039	1 0 0 0 2	

315. C₄H₇N₂O₄

Glycine dipeptide

RN: MP (°C):
 MW: 147.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.418E+00	2.086E+02	20	B032	1 2 2 1 2	
1.534E+00	2.257E+02	25	B032	1 2 2 1 2	
1.540E+00	2.266E+02	25.1	N024	0 0 0 0 0	
1.546E+00	2.275E+02	25.1	N026	0 0 0 0 0	
1.647E+00	2.423E+02	29.80	B032	1 2 2 1 2	

316. C₄H₇N₃O

Creatinine

Kreatinin

RN: 60-27-5

MP (°C): 220.5

MW: 113.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.075E-01	8.004E+01	16	D041	1 0 0 0 1	
7.081E-01	8.010E+01	16	F300	1 0 0 0 2	

317. C₄H₈

1-Butene

α-Butene

Ethylethylene

α-Butylene

1-Butylene

Butene-1

RN: 106-98-9

MP (°C): -185

MW: 56.11

BP (°C): -6.47

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.957E-03	2.220E-01	25	M001	2 1 2 2 2	
1.210E-02	6.791E-01	38	B123	1 2 1 1 2	
1.582E-02	8.876E-01	71	B123	1 2 1 1 2	
2.746E-02	1.541E+00	104	B123	1 2 1 1 2	
3.526E-02	1.979E+00	138	B123	1 2 1 1 2	
3.858E-02	2.165E+00	144.00	B123	1 2 1 1 2	

318. C₄H₈

Isobutylene

2-Methylpropene

RN: 115-11-7

MP (°C): -140.3

MW: 56.11

BP (°C): -6.90

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.687E-03	2.630E-01	25	M001	2 1 2 2 2	

319. C₄H₈Cl₂

2,3-Dichlorobutane

Butane, 2,3-dichloro-

RN: 7581-97-7 **MP (°C):** -80
MW: 127.01 **BP (°C):** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-02	1.817E+00	0	L103	1 0 0 0 2	unit assumed
4.422E-03	5.617E-01	20	L103	1 0 0 0 2	unit assumed
1.464E-03	1.860E-01	30	L103	1 0 0 0 2	unit assumed
1.755E-03	2.230E-01	40	L103	1 0 0 0 2	unit assumed

320. C₄H₈Cl₂O

sym-Dichloroethyl ether

2,2'-Dichlorodiethylether

RN: 111-44-4 **MP (°C):** -50
MW: 143.01 **BP (°C):** 66

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.060E-02	1.010E+01	20	D052	1 1 0 0 0	
7.403E-02	1.059E+01	20	M062	1 0 0 0 2	

321. C₄H₈Cl₂OS

β,β'-Dichlorodiethylsulfoxide

β,β'-Dichlor-diaethylsulfoxid

RN: 5819-08-9 **MP (°C):**
MW: 175.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.854E-02	1.200E+01	20	F300	1 0 0 0 1	

322. C₄H₈Cl₂O₂S

β,β'-Dichlorodiethylsulfone

β,β'-Dichlor-diaethylsulfon

RN: 471-03-4 **MP (°C):**
MW: 191.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.140E-02	6.000E+00	20	F300	1 0 0 0 0	
1.256E-01	2.400E+01	100	F300	1 0 0 0 1	

323. C₄H₈Cl₂S

Mustard gas

Sulfure β'-ethyl dichlore

β,β'-Dichlor-diaethylsulfid

RN: 505-60-2 MP (°C):

MW: 159.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.337E-03	6.900E-01	25	F300	1 0 0 0 1	
3.017E-03	4.800E-01	c	B079	0 0 1 1 1	

324. C₄H₈Cl₃O₄P

Trichlorfon

O,O-Dimethyl (1-hydroxy-2,2,2-trichloroethyl)phosphonate

RN: 52-68-6 MP (°C): 83.5

MW: 257.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.982E-01	1.540E+02	25	M161	1 0 0 0 2	
4.255E-01	1.095E+02	ns	M061	0 0 0 0 2	

325. C₄H₈N₂O₂

Dimethylglyoxime

Dimethylglyoxim

RN: 95-45-4 MP (°C): 240.5

MW: 116.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.167E-03	6.000E-01	20	F300	1 0 0 0 0	
3.100E-02	3.600E+00	80	F300	1 0 0 0 1	
5.081E-02	5.900E+00	100	F300	1 0 0 0 1	

326. C₄H₈N₂O₂

Succinamide

Bersteinsaeure-diamid

RN: 110-14-5 MP (°C): 260

MW: 116.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.858E-02	4.480E+00	15	D041	1 0 0 0 1	
2.842E-02	3.300E+00	15	F300	1 0 0 0 1	
8.534E-01	9.910E+01	100	D041	1 0 0 0 2	
3.445E-04	4.000E-02	c	L055	0 0 0 0 2	
9.463E-03	1.099E+00	h	L055	0 0 0 0 1	
2.818E-02	3.273E+00	ns	R424	0 0 0 0 0	

327. C₄H₈N₂O₃ β -Alanine hydantoic acid β -Uramidopropionic acidGlycine, *N*-(aminocarbonyl)-*N*-methyl-**RN:** 30565-25-4 **MP (°C):****MW:** 132.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-01	2.087E+01	25	M024	1 2 0 1 2	

328. C₄H₈N₂O₃*N*-Nitroso-*N*-methylurethane*N*-Nitroso-*N*-methyl-urethan**RN:** 615-53-2 **MP (°C):****MW:** 132.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-01	3.699E+01	24	M031	1 1 1 1 1	

329. C₄H₈N₂O₃*N*-Glycylglycine

Diglycine

RN: 556-50-3 **MP (°C):** 215**MW:** 132.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E+00	1.656E+02	21	F300	1 0 0 0 2	
1.740E+00	2.299E+02	24.99	B441	0 0 0 0 0	
1.399E+00	1.848E+02	25	G092	2 1 1 1 1	
1.399E+00	1.848E+02	25	G315	0 0 0 0 0	
1.430E+00	1.890E+02	25.1	N027	1 2 2 2 2	
1.512E+00	1.998E+02	ns	M025	0 2 0 1 2	

330. C₄H₈N₂O₃ α -Alanine hydantoic acid

Methylhydantoic acid

RN: 77340-50-2 **MP (°C):****MW:** 132.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.930E-01	2.550E+01	25	M024	1 2 0 1 2	
1.930E-01	2.550E+01	ns	M025	0 2 0 1 2	

331. C₄H₈N₂O₃

Asparagine

L-Asparagine

L-Asparagin

RN: 70-47-3**MP (°C):** 235**MW:** 132.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.509E-02	8.600E+00	0	F300	1 0 0 0 1	
2.180E-01	2.880E+01	15	D349	2 1 1 2 2	
1.759E-01	2.324E+01	20	B032	1 2 2 1 2	
2.210E-01	2.920E+01	20	D349	2 1 1 2 2	
1.589E-01	2.100E+01	20	F300	1 0 0 0 2	
8.477E-02	1.120E+01	21.5	P045	0 0 2 1 2	
2.226E-01	2.941E+01	25	B032	1 2 2 1 2	
2.260E-01	2.986E+01	25	D349	2 1 1 2 2	
1.709E-01	2.258E+01	25	G315	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N024	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N025	0 0 0 0 0	
1.900E-01	2.510E+01	25.1	N026	0 0 0 0 0	
1.853E-01	2.449E+01	25.1	N027	1 1 2 2 2	
1.918E-01	2.534E+01	27	D036	0 0 0 0 0	
2.233E-01	2.950E+01	27	D036	0 0 0 0 0	
2.777E-01	3.669E+01	29.80	B032	1 2 2 1 2	
2.604E+00	3.440E+02	98	F300	1 0 0 0 2	
1.817E-01	2.400E+01	ns	D072	0 0 0 0 1	
1.860E-01	2.457E+01	ns	M025	0 2 0 1 2	
1.774E-01	2.344E+01	rt	D021	0 0 1 1 2	

332. C₄H₈N₂O₃.H₂O

L-Asparagine monohydrate

Asparagine, monohydrate, L-

RN: 5794-13-8 **MP (°C):** 234**MW:** 150.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-01	2.902E+01	25	D041	1 0 0 0 2	
1.858E-01	2.790E+01	25	O316	1 0 1 2 2	
1.853E-01	2.781E+01	25	O316	1 0 1 2 2	
1.293E+00	1.941E+02	75	D041	1 0 0 0 2	

333. C₄H₈N₄O₂

N,N'-Dinitrosopiperazine

Dinitrosopiperazine

RN: 140-79-4 **MP (°C):****MW:** 144.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-02	5.765E+00	24	D083	2 0 0 0 1	

334. C₄H₈O

2-Butyraldehyde
Butyraldehyde
Butyraldehyd
n-Butanal

RN: 123-72-8 **MP (°C):** -96
MW: 72.11 **BP (°C):** 75

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-01	3.568E+01	20	D041	1 0 0 0 1	
4.993E-01	3.600E+01	20	F300	1 0 0 0 1	
9.694E-01	6.990E+01	25	A049	1 0 0 0 2	
9.194E-01	6.629E+01	25	B060	2 0 1 1 1	
5.077E-01	3.661E+01	38	J020	2 2 2 1 1	

335. C₄H₈O

Ethyl vinyl ether
Aethyl-vinyl-aether

RN: 109-92-2 **MP (°C):** -115.0
MW: 72.11 **BP (°C):** 35

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-01	1.002E+01	37	E028	1 1 2 2 2	

336. C₄H₈O

Isobutyraldehyde
2-Methyl propanal

RN: 78-84-2 **MP (°C):** -66
MW: 72.11 **BP (°C):** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E+00	8.413E+01	20	M146	1 2 2 2 2	
1.234E+00	8.900E+01	25	A049	1 0 0 0 0	

337. C₄H₈O

Methyl ethyl ketone
Butanon-(2)

RN: 78-93-3 **MP (°C):** -87
MW: 72.11 **BP (°C):** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		0	C423	0 0 0 0 0	
5.780E+00	4.168E+02	4	C423	0 0 0 0 0	
4.338E+00	3.128E+02	10	C423	0 0 0 0 0	
1.015E+00	7.322E+01	20	A075	1 0 0 0 1	

(continued)

337. C₄H₈O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E+00	2.038E+02	20	D052	1 1 0 0 2	
2.922E+00	2.107E+02	20	E019	1 0 1 1 2	
2.399E+00	1.730E+02	20	F300	1 0 0 0 2	
2.977E+00	2.146E+02	20	G030	1 2 0 0 2	
5.020E+00	3.620E+02	20	P040	0 0 0 0 0	
2.931E+00	2.114E+02	25	A094	1 0 0 0 2	
3.302E+00	2.381E+02	25	A356	0 0 0 0 0	
2.931E+00	2.114E+02	25	B060	2 0 1 1 1	
3.732E+00	2.691E+02	25	C435	0 0 0 0 0	
3.130E+00	2.257E+02	25	F044	1 0 0 0 2	
2.824E+00	2.036E+02	25	G030	1 2 0 0 2	
2.657E+00	1.916E+02	25	J005	1 0 2 1 2	
6.112E+00	4.407E+02	25	K105	2 0 0 0 2	
2.912E+00	2.100E+02	25	M136	2 0 0 0 2	
2.912E+00	2.100E+02	25	M139	2 0 0 0 2	
2.720E+00	1.961E+02	25	N309	1 0 0 0 2	
2.756E+00	1.987E+02	25	O028	2 2 2 2 2	
2.556E+00	1.843E+02	25	P055	1 0 0 0 1	
2.774E+00	2.000E+02	25	R320	1 0 1 1 2	
2.690E+00	1.940E+02	30	G030	1 2 0 0 2	
1.703E+00	1.228E+02	30	R319	2 2 2 1 2	
2.900E+00	2.091E+02	35	A356	0 0 0 0 0	
2.969E+00	2.141E+02	35	C309	2 2 2 2 1	
2.538E+00	1.830E+02	38	J020	2 0 2 1 2	
7.726E-01	5.571E+01	40	A075	1 0 0 0 1	
2.723E+00	1.964E+02	45	A356	0 0 0 0 0	
2.615E+00	1.885E+02	45	C309	2 2 2 2 1	
6.257E+00	4.512E+02	45	K105	2 0 0 0 2	
6.855E-01	4.943E+01	60	A075	1 0 0 0 1	
6.319E+00	4.556E+02	60	K105	2 0 0 0 2	
6.352E-01	4.580E+01	70	A075	1 0 0 0 1	
3.453E+00	2.490E+02	70	P040	0 0 0 0 0	
2.219E+00	1.600E+02	90	F300	1 0 0 0 1	
3.627E+00	2.615E+02	100	P040	0 0 0 0 0	
6.844E+00	4.935E+02	140	P040	0 0 0 0 0	
3.334E+00	2.404E+02	ns	C309	2 2 2 2 1	
+1.89E+00	+1.36E+02	ns	S460	0 0 0 0 0	

338. C₄H₈O

Tetrahydrofuran

1,4-Epoxybutane

Butylene oxide

RN: 109-99-9

MP (°C): -108.0

MW: 72.11

BP (°C): 66.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.498E+00	3.243E+02	72.2	M347	2 2 2 1 2	
4.504E+00	3.248E+02	72.25	M347	2 2 2 1 2	

(continued)

338. C₄H₈O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E+00	3.271E+02	72.3	M347	2 2 2 1 2	
4.251E+00	3.065E+02	73.4	M347	2 2 2 1 2	
4.019E+00	2.898E+02	75.4	M347	2 2 2 1 2	
3.678E+00	2.652E+02	78.6	M347	2 2 2 1 2	
3.595E+00	2.593E+02	78.9	M347	2 2 2 1 2	
3.378E+00	2.436E+02	83.3	M347	2 2 2 1 2	
3.257E+00	2.349E+02	87.9	M347	2 2 2 1 2	
3.217E+00	2.320E+02	89.5	M347	2 2 2 1 2	
3.118E+00	2.248E+02	92.9	M347	2 2 2 1 2	
3.042E+00	2.194E+02	102.5	M347	2 2 2 1 2	
3.042E+00	2.194E+02	110.5	M347	2 2 2 1 2	
3.118E+00	2.248E+02	119.3	M347	2 2 2 1 2	
3.257E+00	2.349E+02	127.8	M347	2 2 2 1 2	
3.595E+00	2.593E+02	132.9	M347	2 2 2 1 2	
3.998E+00	2.883E+02	136.1	M347	2 2 2 1 2	
4.067E+00	2.933E+02	136.5	M347	2 2 2 1 2	
4.617E+00	3.329E+02	137.1	M347	2 2 2 1 2	
6.934E+00	5.000E+02	rt	B066	0 2 0 0 2	

339. C₄H₈O₂

Ethyl acetate

Aethylacetat

Essigsaeureaethyl ester

RN: 141-78-6 MP (°C): -83
 MW: 88.11 BP (°C): 77

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.941E-01	8.759E+01	0	B108	1 2 0 1 1	
1.097E+00	9.666E+01	0	B108	1 2 0 1 2	
1.919E+00	1.691E+02	0	C423	0 0 0 0 0	
1.069E+00	9.420E+01	0	G062	1 2 2 2 2	
1.032E+00	9.091E+01	0	M088	2 0 0 0 1	
1.144E+00	1.008E+02	0	M111	1 0 1 1 2	
1.054E+00	9.290E+01	4	C423	0 0 0 0 0	
8.297E-01	7.310E+01	10	C423	0 0 0 0 0	
9.333E-01	8.223E+01	10	G062	1 2 2 2 2	
1.001E+00	8.817E+01	10	M111	1 0 1 1 2	
9.944E-01	8.762E+01	10.0	K079	1 0 0 0 2	
8.698E-01	7.664E+01	15	M088	2 0 0 0 1	
9.419E-01	8.299E+01	15	M111	1 0 1 1 2	
8.329E-01	7.339E+01	17.0	G101	1 2 1 1 2	
8.718E-01	7.681E+01	20	A016	1 2 1 1 2	
8.212E-01	7.236E+01	20	B108	1 2 0 1 1	
8.795E-01	7.749E+01	20	B108	1 2 0 1 2	
7.346E-01	6.472E+01	20	D052	1 1 0 0 2	
9.556E-01	8.419E+01	20	E002	1 0 0 0 2	
7.310E-01	6.441E+01	20	F001	1 0 1 2 2	

(continued)

339. C₄H₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.932E-01	7.870E+01	20	F300	1 0 0 0 2	
8.920E-01	7.860E+01	20	M111	1 0 1 1 2	
7.300E-01	6.432E+01	20	M171	1 0 0 0 1	
7.732E-01	6.812E+01	20	M348	2 2 1 1 2	
9.200E-01	8.106E+01	20	S006	1 0 0 0 1	
8.778E-01	7.734E+01	20.0	K079	1 0 0 0 2	
8.708E-01	7.672E+01	20.40	A016	1 2 1 1 2	
8.417E-01	7.416E+01	25	A016	1 2 1 1 2	
9.084E-01	8.004E+01	25	A094	1 0 0 0 1	
8.243E-01	7.263E+01	25	A326	1 2 0 1 1	
5.396E-02	4.755E+00	25	B004	0 0 0 0 0	sic
9.084E-01	8.004E+01	25	B060	2 0 1 1 1	
9.180E-01	8.088E+01	25	B092	2 1 1 1 2	
9.080E-01	8.000E+01	25	B304	2 0 2 2 0	
7.321E-01	6.450E+01	25	C435	0 0 0 0 0	
8.988E-01	7.919E+01	25	D425	0 0 0 0 0	
7.810E-01	6.881E+01	25	G062	1 2 2 2 2	
7.977E-01	7.029E+01	25	L062	2 2 0 1 2	
9.847E-01	8.676E+01	25	L319	1 0 2 1 2	
8.485E-01	7.476E+01	25	M111	1 0 1 1 2	
8.310E-01	7.322E+01	25	P055	1 0 0 0 1	
8.222E-01	7.244E+01	25.0	K079	1 0 0 0 2	
8.436E-01	7.433E+01	25.10	A016	1 2 1 1 2	
7.653E-01	6.743E+01	27.0	G101	1 2 1 1 2	
7.603E-01	6.699E+01	27.5	G101	1 2 1 1 2	
8.124E-01	7.158E+01	30	A016	1 2 1 1 2	
8.115E-01	7.149E+01	30	A016	1 2 1 1 2	
7.524E-01	6.629E+01	30	M088	2 0 0 0 1	
8.124E-01	7.158E+01	30	M111	1 0 1 1 2	
7.524E-01	6.629E+01	30	S357	1 2 1 0 2	
7.889E-01	6.951E+01	30.0	K079	1 0 0 0 2	
7.800E-01	6.873E+01	34	A016	1 2 1 1 2	
7.810E-01	6.881E+01	35	A016	1 2 1 1 2	
7.791E-01	6.864E+01	35	M111	1 0 1 1 2	
8.170E-01	7.198E+01	37	E028	1 0 1 1 2	
7.077E-01	6.235E+01	37	G062	1 2 2 2 2	
7.444E-01	6.559E+01	37.0	K079	1 0 0 0 2	
7.425E-01	6.542E+01	38	J020	2 1 2 1 1	
7.574E-01	6.673E+01	39.90	A016	1 2 1 1 2	
7.504E-01	6.612E+01	40	A016	1 2 1 1 2	
7.395E-01	6.516E+01	40	B108	1 2 0 1 2	
7.524E-01	6.629E+01	40	M111	1 0 1 1 2	
6.696E-01	5.900E+01	40	M348	2 2 1 1 2	
7.278E-01	6.412E+01	40.0	K079	1 0 0 0 2	
6.465E-01	5.696E+01	50	G062	1 2 2 2 2	
6.722E-01	5.923E+01	50.0	K079	1 0 0 0 2	
5.907E-01	5.204E+01	55	M348	2 2 1 1 2	
7.820E-01	6.890E+01	60	B092	2 1 1 1 2	
6.790E-01	5.983E+01	70	A326	1 2 0 1 1	

(continued)

339. C₄H₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.549E-01	4.889E+01	70	M348	2 2 1 1 2	
6.727E-01	5.927E+01	70.4	G101	1 2 1 1 1	
1.156E+00	1.018E+02	.0	K079	1 0 0 0 2	
1.600E-01	1.410E+01	ns	D348	0 0 0 0 0	

340. C₄H₈O₂

Methyl propionate

Methylester propanoic acid

RN: 554-12-1 MP (°C): -87.0

MW: 88.11 BP (°C): 79.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.083E+00	9.545E+01	-2.1	K079	1 0 0 0 2	
1.000E+00	8.811E+01	1.0	K079	1 0 0 0 2	
8.778E-01	7.734E+01	11.5	K079	1 0 0 0 2	
8.500E-01	7.489E+01	14.9	K079	1 0 0 0 2	
8.150E-01	7.181E+01	20	S006	1 0 0 0 2	
8.167E-01	7.195E+01	20.0	K079	1 0 0 0 2	
7.778E-01	6.853E+01	27.1	K079	1 0 0 0 2	
7.667E-01	6.755E+01	32.5	K079	1 0 0 0 2	
7.389E-01	6.510E+01	42.7	K079	1 0 0 0 2	

341. C₄H₈O₂

Isobutyric acid

Isobuttersaeure

RN: 79-31-2 MP (°C): -47

MW: 88.11 BP (°C): 153.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.931E+00	1.701E+02	15.2	P060	1 0 0 0 2	
1.931E+00	1.701E+02	15.2	P060	1 2 0 0 2	
4.171E+00	3.675E+02	17	P060	1 0 0 0 2	
4.171E+00	3.675E+02	17	P060	1 2 0 0 2	
2.619E+00	2.308E+02	17.7	H068	2 0 0 0 1	
1.892E+00	1.667E+02	20	D041	1 0 0 0 0	
1.894E+00	1.669E+02	20	F300	1 0 0 0 2	
3.768E+00	3.320E+02	20.0	P060	1 0 0 0 2	
3.768E+00	3.320E+02	20.0	P060	1 2 0 0 2	
3.732E+00	3.289E+02	20.1	P060	1 0 0 0 2	
3.732E+00	3.289E+02	20.1	P060	1 2 0 0 2	
2.255E+00	1.987E+02	20.2	P060	1 2 0 0 2	
2.255E+00	1.987E+02	20.25	P060	1 0 0 0 2	
2.367E+00	2.085E+02	20.9	P060	1 0 0 0 2	
2.363E+00	2.082E+02	20.9	P060	1 2 0 0 2	
3.363E+00	2.963E+02	21.2	P060	1 2 0 0 2	
3.363E+00	2.963E+02	21.2	P060	1 0 0 0 2	

(continued)

341. C₄H₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.161E+00	2.785E+02	21.5	P060	1 2 0 0 2	
3.161E+00	2.785E+02	21.5	P060	1 0 0 0 2	
2.500E+00	2.203E+02	21.5	P060	1 2 0 0 2	
2.500E+00	2.203E+02	21.5	P060	1 0 0 0 2	
3.240E+00	2.855E+02	21.7	P060	1 2 0 0 2	
3.001E+00	2.644E+02	21.76	P060	1 0 0 0 2	
3.003E+00	2.645E+02	21.79	P060	1 0 0 0 2	
2.831E+00	2.495E+02	21.8	P060	1 2 0 0 2	
2.831E+00	2.495E+02	21.89	P060	1 0 0 0 2	
2.709E+00	2.387E+02	21.9	P060	1 0 0 0 2	
2.709E+00	2.387E+02	21.9	P060	1 2 0 0 2	

342. C₄H₈O₂

3-Hydroxytetrahydrofuran
(RS)-3-Hydroxytetrahydrofuran

Tetrahydro-3-furanol

(±)-3-Hydroxytetrahydrofuran

3-Hydroxyoxolane

RN: 453-20-3 MP (°C): <25

MW: 88.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.675E+00	5.000E+02	rt	B066	0 2 0 0 2	

343. C₄H₈O₂

Butyric acid

Buttersaeure

n-Butyric acid

RN: 107-92-6 MP (°C): -7.9

MW: 88.11 BP (°C): 163.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.943E-02	2.593E+00	1.13	H068	2 0 0 0 1	
1.149E-01	1.012E+01	25	B004	0 0 0 0 0	

344. C₄H₈O₂

1,4-Dioxane

1,4-Dioxan

Dioxane

RN: 123-91-1 MP (°C): 11.8

MW: 88.11 BP (°C): 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>9.08E+00	>8.00E+02	25	B019	1 0 1 2 0	

345. C₄H₈O₂

Propyl formate

Ameisensaeure-propylester

Propyl methanoate

n-Propyl formate

RN: 110-74-7 MP (°C): -93

MW: 88.11 BP (°C): 81

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.222E-01	3.720E+01	-1.0	K079	1 0 0 0 2	
3.861E-01	3.402E+01	4.0	K079	1 0 0 0 2	
3.722E-01	3.280E+01	6.0	K079	1 0 0 0 2	
3.444E-01	3.035E+01	12.5	K079	1 0 0 0 2	
3.220E-01	2.837E+01	20	S006	1 0 0 0 2	
3.272E-01	2.883E+01	20.0	K079	1 0 0 0 2	
2.497E-01	2.200E+01	22	F300	1 0 0 0 1	
3.161E-01	2.785E+01	30.0	K079	1 0 0 0 2	
2.880E-01	2.537E+01	32.5	N014	0 0 0 0 0	
3.083E-01	2.717E+01	34.0	K079	1 0 0 0 2	
2.972E-01	2.619E+01	45.0	K079	1 0 0 0 2	

346. C₄H₈Br

Isobutyl bromide

1-Bromo-2-methylpropane

RN: 78-77-3 MP (°C): -119

MW: 137.03 BP (°C): 91.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	5.070E-01	18	F001	1 0 1 0 2	
3.722E-03	5.100E-01	18	F300	1 0 0 0 1	

347. C₄H₈Br*n*-Butyl bromide

Bromobutane

RN: 109-65-9 MP (°C): -112

MW: 137.03 BP (°C): 101.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	5.892E-01	16	F001	1 0 1 0 2	
4.300E-03	5.892E-01	17	S006	1 0 0 0 1	
<1.46E-03	<2.00E-01	25	B019	1 0 1 2 0	
4.500E-03	6.166E-01	25	K012	1 0 0 0 1	
6.340E-03	8.687E-01	25	M342	1 0 1 1 2	
4.434E-03	6.076E-01	30	G029	1 0 2 2 2	
4.500E-02	6.166E+00	ns	H307	0 0 0 0 0	

348. C₄H₉Cl

Isobutyl chloride

Isobutylchlorid

RN: 513-36-0

MP (°C): -131

MW: 92.57

BP (°C): 68

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	9.257E-01	12.5	F001	1 0 1 2 2	
9.722E-03	9.000E-01	12.50	F300	2 0 0 0 1	

349. C₄H₉Cl*n*-Butyl chloride

1-Chlorobutane

RN: 109-69-3

MP (°C): -123.0

MW: 92.57

BP (°C): 78.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-03	6.665E-01	12.5	F001	1 0 1 0 2	
7.130E-02	6.600E+00	12.50	F300	1 0 0 0 1	
8.000E-03	7.406E-01	25	K012	1 0 0 0 0	
9.430E-03	8.729E-01	25	M342	1 0 1 1 2	
7.557E-03	6.995E-01	ns	N034	0 0 0 0 1	

350. C₄H₉Cl*sec*-Butyl chloride

2-Chlorobutane

RN: 78-86-4

MP (°C): -140

MW: 92.57

BP (°C): 68

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.079E-02	9.990E-01	25	N034	1 0 0 0 0	

351. C₄H₉Cl*tert*-Butyl chloride

2-Chloro-2-methylpropane

RN: 507-20-0

MP (°C): -26.5

MW: 92.57

BP (°C): 51.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.180E-02	7.572E+00	.99	C064	2 2 1 1 2	
6.620E-02	6.128E+00	5.00	C064	2 2 1 1 2	
3.110E-02	2.879E+00	14.90	C064	2 2 1 1 2	

352. C₄H₉I

Iodobutane

n-Butyl iodide

RN: 542-69-8 **MP (°C):** -103
MW: 184.02 **BP (°C):** 130.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	2.024E-01	17.5	F001	1 0 1 0 2	
1.100E-03	2.024E-01	17.5	S006	1 0 0 0 1	
1.100E-03	2.024E-01	20	M171	1 0 0 0 1	
1.700E-03	3.128E-01	25	K012	1 0 0 0 1	

353. C₄H₉NO*N,N*-Dimethylacetamide

Acetdimethylamide

U-5954

RN: 127-19-5 **MP (°C):** -20
MW: 87.12 **BP (°C):** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.071E+00	5.289E+02	4.50	C022	1 2 0 0 2	

354. C₄H₉NO

Butyramide

n-Butyramide

RN: 541-35-5 **MP (°C):** 116
MW: 87.12 **BP (°C):** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E+00	1.708E+02	6	H059	0 0 0 0 0	
2.190E+00	1.908E+02	16	H059	0 0 0 0 0	
2.640E+00	2.300E+02	25	H059	0 0 0 0 0	

355. C₄H₉NO₂ γ -Aminobutyric acid γ -Amino-buttersäure γ -Amino-*n*-butyric acid

RN: 56-12-2 **MP (°C):**
MW: 103.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.261E+01	1.300E+03	25	M029	2 2 2 2 2	

356. C₄H₉NO₂

Propyl carbamate

n-Propyl carbamate

RN: 627-12-3 **MP (°C):** 60
MW: 103.12 **BP (°C):** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E+00	2.001E+02	37	H006	1 2 2 1 2	

357. C₄H₉NO₂DL- α -Aminobutyric acid

DL-2-Aminobutyric acid

RN: 2835-81-6 **MP (°C):** 304
MW: 103.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.121E+00	2.188E+02	20	D041	1 0 0 0 1	
1.615E+00	1.665E+02	25	K031	2 1 2 1 2	

358. C₄H₉NO₂ β -Aminobutyric acid β -Amino-*n*-butyric acid

RN: 2835-82-7 **MP (°C):** 193
MW: 103.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+01	1.250E+03	25	M029	2 2 2 2 2	

359. C₄H₉NO₂ α -Aminoisobutyric acid α -Amino-isobuttersaeure α -Aminoisobutyric acid

2-Methylalanine

RN: 62-57-7 **MP (°C):**
MW: 103.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E+00	1.371E+02	25	C018	0 0 0 0 0	
1.170E+00	1.206E+02	25	D041	1 0 0 0 2	
1.482E+00	1.528E+02	25	M029	2 2 2 2 2	
1.759E+00	1.814E+02	25	M097	2 2 2 2 2	

360. C₄H₉NO₂

1-Nitrobutane

Butane, 1-nitro-

RN: 627-05-4

MP (°C): -81

MW: 103.12

BP (°C): 152.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-02	3.609E+00	25	K012	1 0 0 0 1	

361. C₄H₉NO₂

N-Methylurethane

Ethyl methylaminoformate

Ethyl methylcarbamate

Ethyl N-methyl carbamate

Methyl urethane

N-Methylurethane

RN: 105-40-8

MP (°C):

MW: 103.12

BP (°C): 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+3.97E+00	+4.10E+02	ns	S460	0 0 0 0 0	

362. C₄H₉NO₂

α-Aminobutyric acid

2-Aminobutanoic acid

α-Amino-n-butyric acid

Butanoic acid

RN: 80-60-4

MP (°C): 304

MW: 103.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.845E+00	1.902E+02	25	A048	1 1 1 1 2	form A
1.624E+00	1.674E+02	25	A048	1 1 1 1 2	form B
1.800E+00	1.856E+02	25	C018	0 0 0 0 0	
1.800E+00	1.856E+02	25	E015	1 2 1 1 2	
2.041E+00	2.105E+02	25	M029	2 2 2 2 2	
1.852E+00	1.910E+02	35	A048	1 1 1 1 2	form A
1.771E+00	1.826E+02	35	A048	1 1 1 1 2	form B
1.931E+00	1.991E+02	45	A048	1 1 1 1 2	form A
1.917E+00	1.977E+02	45	A048	1 1 1 1 2	form B

363. C₄H₉NO₃

L-Threonine

Threonine

RN: 72-19-5**MP (°C):** 270**MW:** 119.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.606E-01	9.060E+01	20	B032	1 2 2 1 2	
8.139E-01	9.695E+01	25	B032	1 2 2 1 2	
7.346E-01	8.751E+01	25	G315	0 0 0 0 0	
8.202E-01	9.770E+01	25.1	N024	0 0 0 0 0	
8.227E-01	9.800E+01	25.1	N026	0 0 0 0 0	
7.493E-01	8.925E+01	25.1	N027	1 1 2 2 2	
8.168E-01	9.730E+01	27	D036	0 0 0 0 0	
8.695E-01	1.036E+02	29.80	B032	1 2 2 1 2	

364. C₄H₉NO₃DL-*allo*-Threonine

DL-Allothreonine

RN: 144-98-9**MP (°C):****MW:** 119.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.024E+00	1.220E+02	25	D041	1 0 0 0 2	
1.987E+00	2.366E+02	80	D041	1 0 0 0 2	

365. C₄H₉NO₃

DL-Threonine

(±)-Threonine

RN: 80-68-2**MP (°C):** 244**MW:** 119.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.405E+00	1.674E+02	25	D041	1 0 0 0 2	
2.979E+00	3.548E+02	80	D041	1 0 0 0 1	

366. C₄H₉NO₃

Butyl nitrate

N-Butyl nitrate

RN: 928-45-0**MP (°C):****MW:** 119.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-03	7.743E-01	25	K012	1 0 0 0 1	

367. C₄H₉N₃O₂

Creatine

Kreatin

RN: 57-00-1

MP (°C): 219

MW: 131.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.222E-02	1.078E+01	10	D041	1 0 0 0 2	
1.016E-01	1.332E+01	18	D041	1 0 0 0 2	
1.014E-01	1.330E+01	18	F300	1 0 0 0 2	

368. C₄H₉O₅P γ -Phosphono-*n*-butyric acid

4-Phosphonobutyric acid

Phosphonic acid, (3-carboxypropyl)-

Butyric acid, 4-phosphono-

RN: 4378-43-2

MP (°C):

MW: 168.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.739E+00	2.923E+02	0	N028	1 0 0 0 2	
2.068E+00	3.477E+02	20	N028	1 0 0 0 2	

369. C₄H₁₀

Isobutane

1,1-Dimethylethane

2-Methylpropane

Trimethylmethane

Purifrigor iso 3.5

R 600 α

RN: 75-28-5

MP (°C): -159

MW: 58.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~5.68E-03	~3.30E-01	17	F300	1 0 0 0 0	
8.413E-04	4.890E-02	25	M001	2 1 2 2 2	
8.413E-04	4.890E-02	25	M002	2 1 2 2 2	

370. C₄H₁₀

Butane

n-Butane

Diethyl

HC 600

Liquefied petroleum gas

R 600 (alkane)

RN: 106-97-8 MP (°C): -138

MW: 58.12 BP (°C): -0.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.138E-03	1.824E-01	3	R063	0 0 0 0 0	
3.210E-03	1.866E-01	4	K031	2 1 2 1 2	
2.622E-03	1.524E-01	6	R063	0 0 0 0 0	
2.314E-03	1.345E-01	9	R063	0 0 0 0 0	
1.886E-03	1.096E-01	14	R063	0 0 0 0 0	
1.461E-03	8.492E-02	19.8	G058	1 0 0 0 2	
1.260E-03	7.324E-02	25	K031	2 1 2 1 2	
1.056E-03	6.140E-02	25	M001	2 1 2 2 2	
1.056E-03	6.140E-02	25	M002	2 1 2 2 2	
1.056E-03	6.140E-02	25	M040	1 0 0 1 2	
2.773E-02	1.612E+00	38	R078	0 0 0 0 0	
6.600E-04	3.836E-02	50	K031	2 1 2 1 2	
1.159E-01	6.735E+00	71	R078	0 0 0 0 0	
4.596E-01	2.671E+01	104	R078	0 0 0 0 0	
1.370E+00	7.965E+01	138	R078	0 0 0 0 0	

371. C₄H₁₀NO₃PS

Acephate

Orthene

Acetylphosphoramidothioic acid O,S-dimethyl ester

RN: 30560-19-1 MP (°C): 85.5

MW: 183.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.151E+00	3.939E+02	rt	M161	0 0 0 0 1	

372. C₄H₁₀N₂O

N-Nitrosodiethylamine

Diethyl nitrosamine

RN: 55-18-5 MP (°C):

MW: 102.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E+00	1.062E+02	24	D083	2 0 0 0 2	

373. C₄H₁₀O

Methyl propyl ether

1-Methoxypropane

RN: 557-17-5

MP (°C): <25

MW: 74.12

BP (°C): 38.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.154E-01	5.303E+01	0	B002	2 1 1 2 2	
4.939E-01	3.661E+01	10	B002	2 1 1 2 2	
4.436E-01	3.288E+01	15	B002	2 1 1 2 2	
4.183E-01	3.101E+01	20	B002	2 1 1 2 2	
3.993E-01	2.960E+01	25	B002	2 1 1 2 2	

374. C₄H₁₀O*tert*-Butyl alcohol

2-Methyl-2-propanol

tert-Butanol

RN: 75-65-0

MP (°C): 25.6

MW: 74.12

BP (°C): 82.41

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.712E-02	6.458E+00	79.40	B165	1 0 1 1 2	

375. C₄H₁₀O*n*-Butyl alcohol

Butanol-(1)

n-Butanol

1-Butanol

Butyl alcohol

n-Butyl alcohol

RN: 71-36-3

MP (°C): -90

MW: 74.12

BP (°C): 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.262E+00	9.355E+01	0	E029	1 2 0 1 2	
1.176E+00	8.717E+01	0	M095	2 2 1 2 2	
1.176E+00	8.717E+01	5	H003	1 2 1 1 2	
1.077E+00	7.987E+01	10	E029	1 2 0 1 2	
1.104E+00	8.181E+01	10	H003	1 2 1 1 2	
6.015E+00	4.459E+02	13.0	J012	1 2 0 1 2	
1.024E+00	7.587E+01	15	H003	1 2 1 1 2	
1.034E+00	7.664E+01	15	M095	2 2 1 2 2	
9.190E-01	6.812E+01	18	F001	1 0 1 0 2	
8.634E-01	6.400E+01	18	F300	1 0 0 0 1	
7.396E-01	5.482E+01	20	A075	1 0 0 0 1	
9.762E-01	7.236E+01	20	D040	2 2 1 1 2	

(continued)

375. C₄H₁₀O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.993E-01	7.407E+01	20	D052	1 1 0 0 0	
9.482E-01	7.029E+01	20	E029	1 2 0 1 2	
9.773E-01	7.244E+01	20	H003	1 2 1 1 2	
6.302E-01	4.671E+01	20	L084	1 1 1 1 1	
1.040E+00	7.709E+01	20	M312	1 0 0 0 1	
8.270E-01	6.130E+01	23	D063	1 0 1 2 2	
1.021E+00	7.567E+01	23.5	D063	1 0 0 2 2	
9.983E-01	7.400E+01	25	A049	1 0 1 0 0	
1.125E+00	8.341E+01	25	B019	1 0 1 2 0	
9.645E-01	7.149E+01	25	B060	2 0 1 1 1	
1.000E+00	7.412E+01	25	F044	1 0 0 0 0	EFG
8.708E-01	6.455E+01	25	F325	1 2 0 1 1	
9.200E-01	6.819E+01	25	G075	1 0 1 0 1	
9.237E-01	6.847E+01	25	H003	1 2 1 1 2	
9.307E-01	6.899E+01	25	H028	2 0 2 0 2	
1.070E+00	7.931E+01	25	K012	1 0 0 0 2	
9.700E-01	7.190E+01	25	K025	2 2 1 1 1	
8.867E-01	6.572E+01	25	L322	1 1 2 2 1	
8.904E-01	6.600E+01	25	M136	2 0 0 0 1	
8.904E-01	6.600E+01	25	M139	2 0 0 0 1	
8.826E-01	6.542E+01	25.0	P077	1 1 1 1 1	
8.234E-01	6.103E+01	26	O012	1 2 1 1 2	
8.826E-01	6.542E+01	27	R319	2 2 2 1 1	
5.976E+00	4.429E+02	29.82	J012	1 2 0 1 2	
8.944E-01	6.629E+01	30	D040	2 2 1 1 2	
8.897E-01	6.594E+01	30	E029	1 2 0 1 2	
8.920E-01	6.612E+01	30	F053	1 0 2 0 2	
8.920E-01	6.612E+01	30	H003	1 2 1 1 2	
8.838E-01	6.551E+01	30.0	H043	2 2 1 1 2	
8.625E-01	6.393E+01	35	H003	1 2 1 1 2	
9.061E-01	6.716E+01	38	J020	2 0 2 1 1	
8.471E-01	6.279E+01	38	M125	1 1 1 1 1	
5.933E-01	4.398E+01	40	A075	1 0 0 0 1	
8.353E-01	6.191E+01	40	D040	2 2 1 1 2	
8.495E-01	6.297E+01	40	E029	1 2 0 1 2	
8.353E-01	6.191E+01	40	H003	1 2 1 1 2	
8.234E-01	6.103E+01	45	M095	2 2 1 2 2	
8.293E-01	6.147E+01	50	E029	1 2 0 1 2	
8.186E-01	6.068E+01	50	H003	1 2 1 1 2	
7.756E-01	5.749E+01	50	O012	1 2 1 1 2	
5.837E+00	4.327E+02	58.50	J012	1 2 0 1 2	
5.064E-01	3.754E+01	60	A075	1 0 0 0 1	
8.258E-01	6.121E+01	60	E029	1 2 0 1 2	
8.258E-01	6.121E+01	60	H003	1 2 1 1 2	
5.064E-01	3.754E+01	70	A075	1 0 0 0 1	
8.436E-01	6.253E+01	70	E029	1 2 0 1 2	
8.850E-01	6.560E+01	70	F001	1 0 1 0 2	
8.507E-01	6.306E+01	70	H003	1 2 1 1 2	

(continued)

375. C₄H₁₀O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-01	4.943E+01	75	L084	1 1 1 1 1	
8.590E-01	6.367E+01	75	M095	2 2 1 2 1	
8.708E-01	6.455E+01	80	E029	1 2 0 1 2	
9.460E-01	7.012E+01	80	F001	1 0 1 0 2	
8.696E-01	6.446E+01	80	H003	1 2 1 1 2	
9.412E-01	6.977E+01	90	E029	1 2 0 1 2	
1.054E+00	7.813E+01	90	F001	1 0 1 0 2	
9.762E-01	7.236E+01	90	M095	2 2 1 2 1	
1.084E+00	8.038E+01	97.90	H003	1 2 1 1 2	
1.101E+00	8.164E+01	98.3	R072	2 2 2 1 2	
4.900E+00	3.632E+02	100	E029	1 2 0 1 2	
1.228E+00	9.102E+01	100	F001	1 0 1 0 2	
1.204E+00	8.925E+01	105	M095	2 2 1 2 1	
1.342E+00	9.950E+01	110	E029	1 2 0 1 2	
1.473E+00	1.092E+02	110	F001	1 0 1 0 2	
1.523E+00	1.129E+02	114.50	H003	1 2 1 1 2	
1.600E+00	1.186E+02	116.90	H003	1 2 1 1 2	
1.805E+00	1.338E+02	120	E029	1 2 0 1 2	
2.223E+00	1.648E+02	123.30	H003	1 2 1 1 2	
2.890E+00	2.142E+02	124.80	H003	1 2 1 1 2	
2.567E+00	1.903E+02	125	E029	1 2 0 1 2	
3.334E+00	2.471E+02	125.10	H003	1 2 1 1 2	
3.148E+00	2.334E+02	125.20	H003	1 2 1 1 2	
9.307E-01	6.899E+01	ns	A406	0 0 0 0 1	
7.920E-01	5.871E+01	ns	D348	0 0 0 0 0	
9.744E-01	7.222E+01	ns	L003	0 0 2 1 2	
9.033E+00	6.695E+02	ns	M314	2 1 2 1 2	

376. C₄H₁₀O

Methyl isopropyl ether

2-Methoxypropane

RN: 598-53-8 MP (°C): <25

MW: 74.12 BP (°C): 32

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.193E+00	8.842E+01	10	B002	2 1 1 2 2	
1.068E+00	7.919E+01	15	B002	2 1 1 2 2	
9.295E-01	6.890E+01	20	B002	2 1 1 2 2	
8.234E-01	6.103E+01	25	B002	2 1 1 2 2	
8.437E-01	6.254E+01	ns	J300	0 0 0 0 0	

377. C₄H₁₀O

Isobutyl alcohol

2-Methyl-1-propanol

RN: 78-83-1 **MP (°C):** -108
MW: 74.12 **BP (°C):** 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.351E+00	1.001E+02	18	F001	1 0 1 2 2	
1.228E+00	9.100E+01	18	F300	1 0 0 0 0	
1.278E+00	9.471E+01	20	M146	1 2 2 2 2	
1.280E+00	9.488E+01	20	M312	1 0 0 0 1	
1.000E+00	7.416E+01	25	A037	2 2 2 2 2	
1.226E+00	9.091E+01	25	D052	1 1 0 0 2	
9.529E-01	7.063E+01	25	F050	1 0 0 0 1	
8.967E-01	6.647E+01	25	F317	2 1 1 1 2	
1.045E+00	7.749E+01	29.84	M114	2 2 1 1 1	
9.529E-01	7.063E+01	39.74	M114	2 2 1 1 1	
8.234E-01	6.103E+01	49.64	M114	2 2 1 1 1	
8.590E-01	6.367E+01	59.54	M114	2 2 1 1 1	
9.295E-01	6.890E+01	79.24	M114	2 2 1 1 1	
9.645E-01	7.149E+01	89.14	M114	2 2 1 1 1	
5.168E+00	3.831E+02	90.5	J017	1 0 1 2 2	
5.033E+00	3.730E+02	91.0	J017	1 0 1 2 2	
4.887E+00	3.622E+02	92.0	J017	1 0 1 2 2	
4.871E+00	3.610E+02	92.1	J017	1 0 1 2 2	
4.615E+00	3.421E+02	93.0	J017	1 0 1 2 2	
4.135E+00	3.065E+02	94.3	J017	1 0 1 2 2	
3.820E+00	2.832E+02	95.3	J017	1 0 1 2 2	
1.215E+00	9.008E+01	99.04	M114	2 2 1 1 1	
1.348E+00	9.991E+01	108.94	M114	2 2 1 1 2	
1.708E+00	1.266E+02	118.74	M114	2 2 1 1 2	
2.009E+00	1.489E+02	123.74	M114	2 2 1 1 2	
2.239E+00	1.660E+02	125.64	M114	2 2 1 1 2	
2.415E+00	1.790E+02	128.64	M114	2 2 1 1 2	
2.637E+00	1.955E+02	130.64	M114	2 2 1 1 2	
3.000E+00	2.224E+02	132.64	M114	2 2 1 1 2	
3.527E+00	2.614E+02	134.14	M114	2 2 1 1 2	
1.179E+00	8.740E+01	ns	L003	0 0 2 1 1	

378. C₄H₁₀O

Ethyl ether

Diaethyлаether

Diethyl ether

RN: 60-29-7 **MP (°C):** -116
MW: 74.12 **BP (°C):** 34.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.526E+00	1.131E+02	-3.8	H002	2 0 0 1 2	
1.410E+00	1.045E+02	0	H002	1 0 0 1 2	
1.662E+00	1.232E+02	0	K077	1 2 2 2 2	average of 3
1.338E+00	9.920E+01	7.5	K077	1 2 2 2 2	

(continued)

378. C₄H₁₀O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.263E+00	9.360E+01	8.5	K077	1 2 2 2 2	
1.118E+00	8.291E+01	10	H002	1 0 0 1 2	
1.115E+00	8.265E+01	10	K002	1 2 1 1 2	
1.105E+00	8.190E+01	12	K077	1 2 2 2 2	
9.796E-01	7.261E+01	15	F055	1 2 2 2 2	
1.133E+00	8.400E+01	15	F300	1 0 0 0 1	
9.893E-01	7.333E+01	15	H002	1 0 0 1 2	
9.843E-01	7.296E+01	15	K002	1 2 1 1 2	
8.430E+00	6.249E+02	15	M069	1 0 0 0 2	
1.137E+00	8.430E+01	15	T033	1 2 1 1 2	
1.029E+00	7.630E+01	16	K077	1 2 2 2 2	
8.837E-01	6.550E+01	19	K077	1 2 2 2 2	average
8.696E-01	6.446E+01	20	F055	1 2 2 2 2	
8.703E-01	6.451E+01	20	H002	1 0 0 1 2	
8.684E-01	6.437E+01	20	K002	1 2 1 1 2	
8.353E-01	6.191E+01	20	M345	2 1 1 1 1	
8.341E-01	6.183E+01	20	N038	1 0 0 1 2	
8.769E-03	6.500E-01	21	H337	1 0 1 0 2	sic
1.012E+00	7.502E+01	22	H072	1 0 1 1 2	
9.993E-01	7.407E+01	25	B019	1 0 1 2 0	
7.636E-01	5.660E+01	25	F055	1 2 2 2 2	
8.095E-01	6.000E+01	25	F300	1 0 0 0 1	
7.669E-01	5.684E+01	25	H002	1 0 0 1 2	
7.684E-01	5.696E+01	25	K002	1 2 1 1 2	
8.800E-01	6.523E+01	25	K012	1 0 0 0 1	
6.050E+00	4.484E+02	25	M069	1 0 0 0 2	
8.471E-01	6.279E+01	25	M345	2 1 1 1 1	
8.162E-01	6.050E+01	25	T033	1 2 1 1 2	
1.048E-02	7.770E-01	26	H337	1 0 1 0 2	sic
6.839E-01	5.069E+01	30	H002	1 0 0 1 2	
6.839E-01	5.069E+01	30	K002	1 2 1 1 2	
6.799E-01	5.040E+01	30	K077	1 2 2 2 2	
1.073E-02	7.950E-01	32	H337	1 0 1 0 2	sic
5.950E-01	4.410E+01	37	E022	1 0 1 1 0	
7.120E-01	5.278E+01	37	E028	1 0 1 1 2	
9.484E-03	7.030E-01	37	H337	1 0 1 0 2	sic
6.314E-01	4.680E+01	38	K077	1 2 2 2 2	
9.417E-03	6.980E-01	38.5	H337	1 0 1 0 2	sic
9.808E-03	7.270E-01	40	H337	1 0 1 0 2	sic
5.545E-01	4.110E+01	49	K077	1 2 2 2 2	
5.491E-01	4.070E+01	51.5	K077	1 2 2 2 2	
4.857E-01	3.600E+01	62.5	K077	1 2 2 2 2	
4.600E-01	3.410E+01	65	K077	1 2 2 2 2	
4.209E-01	3.120E+01	66.5	K077	1 2 2 2 2	
4.020E-01	2.980E+01	71	K077	1 2 2 2 2	
3.912E-01	2.900E+01	72	K077	1 2 2 2 2	
3.643E-01	2.700E+01	82	K077	1 2 2 2 2	
1.770E-01	1.312E+01	ns	D348	0 0 0 0 0	
9.412E-01	6.977E+01	ns	R028	0 0 0 0 0	
8.826E-01	6.542E+01	rt	B066	0 2 0 0 0	

379. C₄H₁₀O

sec-Butyl alcohol

DL-sec-Butyl alcohol

DL-Butanol-(2)

sec-DL-Butyl alcohol

RN: 78-92-2 MP (°C): -114

MW: 74.12 BP (°C): 99.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.602E+00	1.929E+02	10.04	M119	2 2 2 2 2	
3.222E+00	2.388E+02	20	A070	1 2 1 0 2	
1.499E+00	1.111E+02	20	D052	1 1 0 0 0	
2.106E+00	1.561E+02	20	E019	1 0 1 1 2	
1.497E+00	1.110E+02	20	F300	1 0 0 0 2	
2.230E+00	1.653E+02	20	M112	2 2 1 1 2	
2.267E+00	1.681E+02	20.04	M119	2 2 2 2 2	
1.348E+00	9.991E+01	25	B019	1 0 1 2 0	
1.057E+00	7.834E+01	25	B060	2 0 1 1 1	
1.699E+00	1.260E+02	25	B165	1 0 1 1 1	
2.048E+00	1.518E+02	27.04	M119	2 2 2 2 2	
2.556E+00	1.894E+02	40	A070	1 2 1 0 2	
1.821E+00	1.349E+02	40	M112	2 0 1 1 2	
1.749E+00	1.297E+02	40.04	M119	2 2 2 2 2	
1.573E+00	1.166E+02	50.04	M119	2 2 2 2 2	
2.167E+00	1.606E+02	60	A070	1 2 1 0 2	
1.657E+00	1.228E+02	60	M112	2 0 1 1 2	
1.531E+00	1.135E+02	60.04	M119	2 2 2 2 2	
1.541E+00	1.143E+02	70.04	M119	2 2 2 2 2	
2.167E+00	1.606E+02	80	A070	1 2 1 0 2	
1.657E+00	1.228E+02	80	M112	2 0 1 1 2	
1.636E+00	1.213E+02	80.04	M119	2 2 2 2 2	
1.760E+00	1.304E+02	85	M112	2 0 1 1 2	
5.107E-02	3.786E+00	87.30	B165	1 0 1 1 2	
1.810E+00	1.342E+02	90.04	M119	2 2 2 2 2	
2.087E+00	1.547E+02	100.04	M119	2 2 2 2 2	
2.602E+00	1.929E+02	110.04	M119	2 2 2 2 2	
1.901E+00	1.409E+02	ns	L003	0 0 2 1 2	

380. C₄H₁₀O₂S

Diethyl sulfone

Diaethylsulfone

RN: 597-35-3 MP (°C): 73

MW: 122.19 BP (°C): 248

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E+00	1.350E+02	16	F300	1 0 0 0 2	

381. C₄H₁₀O₄

DL-Threitol

DL-1,2,3,4-Butanetetrol

RN: 6968-16-7 MP (°C): 90

MW: 122.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.353E+00	8.980E+02	25	C346	0 0 0 0 0	

382. C₄H₁₀O₄

Erythritol

Erythrit

RN: 149-32-6 MP (°C): 121.5

MW: 122.12 BP (°C): 330

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.118E+00	3.808E+02	rt	D021	0 0 1 1 2	
4.995E+00	6.100E+02	rt	F300	0 0 0 0 2	

383. C₄H₁₀S

Ethyl sulfide

1,1'-Thiobisethane

Diethyl thioether

RN: 352-93-2 MP (°C): -100

MW: 90.19 BP (°C): 91

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	3.066E+00	25	K012	1 0 0 0 1	

384. C₄H₁₁N

sec-Butylamine

DL-sec-Butylamine

DL-sec-Butylamin

RN: 13952-84-6 MP (°C):

MW: 73.14 BP (°C): 63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E+00	1.120E+02	20	F300	1 0 0 0 2	

385. C₄H₁₁N*n*-Butylamine*n*-Butylamin

1-Aminobutane

RN: 109-73-9 **MP (°C):** -50
MW: 73.14 **BP (°C):** 78

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.259E-02	2.384E+00	25	B004	0 0 0 0 0	

386. C₄H₁₁NO₃

Tromethamine

tris-(Hydroxymethyl)-amino-methan*tris*-(Hydroxymethyl)-aminomethane

2-Amino-2-(hydroxymethyl)-1,3-propanediol

tris(Hydroxymethyl)methylamine

RN: 77-86-1 **MP (°C):** 171.5
MW: 121.14 **BP (°C):** 219.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.564E+00	5.529E+02	15	E305	0 0 0 0 0	
5.766E+00	6.985E+02	25	E305	0 0 0 0 0	
7.160E+00	8.673E+02	35	E305	0 0 0 0 0	

387. C₄H₁₁NO₈P₂

Glyphosine

Polaris

N,N-bis(Phosphonomethyl)glycine

RN: 2439-99-8 **MP (°C):**
MW: 263.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.427E-01	2.480E+02	20	M161	1 0 0 0 2	

388. C₄Cl₆

Hexachloro-1,3-butadiene

Hexachlorobutadiene

RN: 87-68-3 **MP (°C):** -19
MW: 260.76 **BP (°C):** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-06	2.548E-03	20	C113	1 0 2 1 2	
1.917E-05	5.000E-03	20	M068	1 0 0 0 0	
~7.67E-06	~2.00E-03	20	M133	1 0 0 0 0	
1.240E-05	3.233E-03	25	B173	2 0 2 2 2	
7.668E-04	2.000E-01	ns	M061	0 0 0 0 1	

389. C₅H₂Cl₃NO

2,3,5-Trichloro-4-hydroxypyridine

Daxtrom

RN: 1970-40-7 **MP (°C):** 216
MW: 198.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.871E-03	5.697E-01	25	M061	1 0 0 0 1	

390. C₅H₂Cl₃NO

3,5,6-Trichloro-2-pyridinol

3,5,6-Trichloropyridinol

Hydroxy-3,5,6-trichloropyridine

Pyridinone, 3,5,6-trichloro-

RN: 6515-38-4 **MP (°C):**
MW: 198.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.109E-03	2.200E-01	26.70	L095	2 2 1 1 2	
1.109E-03	2.200E-01	ns	K138	0 0 0 0 1	

391. C₅H₃F₃N₂O₂

5-Trifluoromethyl uracil

Trifluorothymine

RN: 54-20-6 **MP (°C):**
MW: 180.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.451E-01	2.613E+01	25	S471	0 0 0 0 0	
1.492E-01	2.687E+01	25	S471	0 0 0 0 0	

392. C₅H₄ClN₅

2-Chloroadenine

1H-Purin-6-amine, 2-chloro-

6-Amino-2-chloropurine

2-Chloro-6-aminopurine

SQ 22982

RN: 1839-18-5 **MP (°C):**
MW: 169.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.895E-05	8.300E-03	25	A336	0 0 0 0 0	

393. C₅H₄N₂O₄

Orotic acid

Vitamin B13

1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid

RN: 65-86-1 MP (°C): 345.5

MW: 156.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.163E-02	1.815E+00	18	B135	1 0 0 0 0	

394. C₅H₄N₂O₄

α,β-Imidazoledicarboxylic acid

4,5-Imidazoledicarboxylic acid

Imidazol-di-carbonsaeure-(4,5)

RN: 570-22-9 MP (°C): 288

MW: 156.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.203E-03	5.000E-01	20	F300	1 0 0 0 1	
8.328E-03	1.300E+00	100	F300	1 0 0 0 1	

395. C₅H₄N₂O₄

5-Carboxyuracil

5-Uracilcarboxylic acid

2,4-Dihydroxypyrimidine-5-carboxylic acid

Uracil-carbonsaeure-(4)

RN: 23945-44-0 MP (°C): 283

MW: 156.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-02	1.800E+00	20	F300	1 0 0 0 1	
7.000E-03	1.093E+00	20	N019	0 0 0 0 0	

396. C₅H₄N₄

Purine

7-Imidazo(4,5-d)pyrimidine

RN: 120-73-0 MP (°C): 216

MW: 120.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.775E+00	3.333E+02	20	A018	1 0 1 1 0	
2.754E+00	3.308E+02	ns	R427	0 0 0 0 0	

397. C₅H₄N₄O

Hypoxanthine
Hypoxanthin

RN: 68-94-0

MP (°C): 150dec

MW: 136.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.139E-03	6.995E-01	19	D041	1 0 0 0 0	
5.143E-03	7.000E-01	23	F300	1 0 0 0 1	
5.290E-03	7.200E-01	25	A337	0 0 0 0 0	
~1.90E-03	~2.59E-01	39.99	T420	0 0 0 0 0	
1.042E-01	1.418E+01	100	D004	0 0 0 0 0	
1.080E-01	1.470E+01	100	F300	1 0 0 0 2	
5.359E-03	7.294E-01	c	D004	0 0 0 0 0	

398. C₅H₄N₄O

Allopurinol

1H-Pyrazolo(3,4-d)pyrimidin-4-ol

Lopurin

RN: 315-30-0

MP (°C): >350

MW: 136.11

BP (°C): 559.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.535E-03	3.450E-01	15	C095	1 0 0 1 2	
3.673E-03	5.000E-01	22	B322	0 0 0 0 0	
3.673E-03	5.000E-01	22	B428	1 2 1 2 1	
3.526E-03	4.800E-01	25	B189	1 0 0 0 1	
4.180E-03	5.690E-01	25	C095	1 0 0 1 2	
6.502E-03	8.850E-01	35	C095	1 0 0 1 2	
7.964E-03	1.084E+00	40	C095	1 0 0 1 2	
3.526E-03	4.800E-01	ns	A351	0 0 0 0 0	
2.475E-03	3.369E-01	ns	B404	0 2 1 1 0	
5.730E-03	7.800E-01	ns	H067	0 0 0 0 0	
7.347E-04	1.000E-01	ns	K444	0 0 0 0 0	

399. C₅H₄N₄O

8-Hydroxypurine

9H-Purin-8-ol

RN: 51953-05-0

MP (°C):

MW: 136.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.048E-02	4.149E+00	20	A022	1 0 0 0 0	

400. C₅H₄N₄O₂

Xanthine

2,6-Dioxopurine

1H-Purine-2,6-dione, 3,7-dihydro-

RN: 69-89-6 **MP (°C):** >300
MW: 152.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.285E-03	4.998E-01	20	D041	1 0 0 0 0	
3.000E-04	4.563E-02	20.99	T418	0 0 0 0 0	
2.458E-04	3.739E-02	21	L015	1 0 1 1 2	
5.246E-04	7.980E-02	37	L015	1 0 1 1 2	
1.312E-02	1.996E+00	100	D041	1 0 0 0 0	

401. C₅H₄N₄O₂.H₂O

Xanthine (monohydrate)

RN: 69-89-6 **MP (°C):** >150dec
MW: 170.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.082E-04	6.944E-02	c	D004	0 0 0 0 0	
3.916E-03	6.662E-01	h	D004	0 0 0 0 0	

402. C₅H₄N₄O₃

Uric acid

Harnsaeure

RN: 69-93-2 **MP (°C):**
MW: 168.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-04	2.000E-02	0	M043	1 0 0 0 0	
7.110E-05	1.195E-02	2.6	M315	1 0 1 1 2	
1.029E-04	1.730E-02	5	R042	1 2 2 1 2	
1.050E-04	1.765E-02	9.3	M315	1 0 1 1 2	
2.379E-04	4.000E-02	10	M043	1 0 0 0 0	
1.326E-04	2.230E-02	14	B116	2 0 1 1 2	
1.190E-04	2.000E-02	20	D041	1 0 0 0 0	
3.569E-04	6.000E-02	20	M043	1 0 0 0 0	
6.610E-04	1.111E-01	22	M145	1 0 1 2 2	intrinsic
1.862E-04	3.130E-02	25	R042	1 2 2 1 2	
2.070E-04	3.480E-02	25.0	M315	1 0 1 1 2	
5.354E-04	9.000E-02	30	F300	1 0 0 0 2	
5.353E-04	8.999E-02	30	M043	1 0 0 0 0	
3.660E-04	6.153E-02	37.0	M315	1 0 1 1 2	
7.137E-04	1.200E-01	40	M043	1 0 0 0 1	
3.753E-04	6.310E-02	40	R042	1 2 2 1 2	
6.280E-04	1.056E-01	50.0	M315	1 0 1 1 2	
6.960E-04	1.170E-01	54	R042	1 2 2 1 2	
1.368E-03	2.299E-01	60	M043	1 0 0 0 1	

(continued)

402. C₅H₄N₄O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.457E-03	2.450E-01	70	F300	1 0 0 0 2	
2.319E-03	3.898E-01	80	M043	1 0 0 0 1	
2.974E-04	5.000E-02	100	D041	1 0 0 0 0	
4.961E-03	8.340E-01	100	F300	1 0 0 0 0	
3.686E-03	6.196E-01	100	M043	1 0 0 0 1	

403. C₅H₄N₄O₃.2H₂O

Uric acid (dihydrate)

RN: 69-93-2 MP (°C):

MW: 204.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.620E-05	1.964E-02	2.6	M315	1 0 1 1 2	
1.420E-04	2.899E-02	9.3	M315	1 0 1 1 2	
3.390E-04	6.920E-02	25.0	M315	1 0 1 1 2	
6.560E-04	1.339E-01	37.0	M315	1 0 1 1 2	
1.440E-03	2.940E-01	50.0	M315	1 0 1 1 2	

404. C₅H₄N₄S

6-Mercaptopurine

6-Purinethiol

Mercaptapurine

Purine-6-thiol

Leukeran

RN: 50-44-2 MP (°C):

MW: 152.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	4.565E-02	4.62	A034	1 1 2 2 0	EFG
8.148E-04	1.240E-01	25	N063	1 1 1 1 2	
4.500E-02	6.848E+00	29.87	A034	1 1 2 2 1	EFG
1.703E-03	2.591E-01	37	H046	1 1 1 1 2	
2.658E-03	4.045E-01	ns	N050	0 1 1 0 0	

405. C₅H₄O₂

Furfural

2-Furaldehyde

Furfurol

RN: 98-01-1 MP (°C): -36

MW: 96.09 BP (°C): 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.620E-01	7.322E+01	10	M099	1 2 0 1 1	
7.816E-01	7.510E+01	16	M099	1 2 0 1 2	
7.869E-01	7.561E+01	17	M099	1 2 0 1 2	
7.976E-01	7.664E+01	20	D052	1 1 0 0 0	

(continued)

405. C₅H₄O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.972E-01	7.660E+01	20	F300	1 0 0 0 2	
7.976E-01	7.664E+01	20	M099	1 2 0 1 1	
7.620E-01	7.322E+01	25	C056	1 2 1 1 1	
8.197E-01	7.877E+01	25	C329	1 2 1 1 1	average
7.709E-01	7.407E+01	25	H338	2 2 1 2 2	
7.976E-01	7.664E+01	25	H340	0 0 0 0 0	
7.441E-01	7.149E+01	25	L062	2 2 1 2 1	
7.709E-01	7.407E+01	25	L320	2 2 1 2 1	
8.242E-01	7.919E+01	25	M099	1 2 0 1 1	
8.347E-01	8.021E+01	27	M099	1 2 0 1 2	
8.347E-01	8.021E+01	27.20	M099	1 2 0 1 2	
8.312E-01	7.987E+01	27.50	M099	1 2 0 1 2	
8.418E-01	8.088E+01	30	M099	1 2 0 1 1	
8.488E-01	8.156E+01	35	H338	2 2 1 2 2	
8.506E-01	8.173E+01	35	L320	2 2 1 2 1	
9.029E-01	8.676E+01	38	G050	1 0 2 1 1	
8.619E-01	8.282E+01	39.50	E037	1 2 2 2 2	
9.029E-01	8.676E+01	40	M099	1 2 0 1 1	
9.289E-01	8.925E+01	44	M099	1 2 0 1 2	
9.804E-01	9.420E+01	50	M099	1 2 0 1 2	
1.023E+00	9.829E+01	52	G050	1 0 2 1 2	
9.306E-01	8.942E+01	53.10	E037	1 2 2 2 2	
4.982E+00	4.787E+02	53.30	E037	1 2 2 2 2	
1.090E+00	1.047E+02	60	M099	1 2 0 1 2	
1.107E+00	1.063E+02	61	M099	1 2 0 1 2	
1.156E+00	1.111E+02	66	G050	1 0 2 1 2	
1.156E+00	1.111E+02	66	M099	1 2 0 1 2	
1.214E+00	1.166E+02	70	M099	1 2 0 1 2	
4.895E+00	4.703E+02	73.60	E037	1 2 2 2 2	
1.318E+00	1.266E+02	79	G050	1 0 2 1 2	
1.342E+00	1.289E+02	80	M099	1 2 0 1 2	
1.361E+00	1.307E+02	85.80	E037	1 2 2 2 2	
1.482E+00	1.424E+02	90	M099	1 2 0 1 2	
1.512E+00	1.453E+02	92	M099	1 2 0 1 2	
1.684E+00	1.618E+02	93	G050	1 0 2 1 2	
4.721E+00	4.536E+02	95.90	E037	1 2 2 2 2	
1.617E+00	1.554E+02	97.90	M099	1 2 0 1 2	

406. C₅H₄O₂S

3-Thenoic acid

Thiophen-carbonsaeure-(3)

RN: 88-13-1 **MP (°C):** 137
MW: 128.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.355E-02	4.300E+00	25	F300	1 0 0 0 1	

407. C₅H₄O₃

2-Furoic acid

Furan-carbon-saeure-(2)

RN: 88-14-2 **MP (°C):** 129.5
MW: 112.09 **BP (°C):** 231

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.227E-01	2.496E+01	5.99	A341	0 0 0 0 0	
2.243E-01	2.514E+01	6.99	A341	0 0 0 0 0	
2.332E-01	2.614E+01	10.49	A341	0 0 0 0 0	
2.498E-01	2.799E+01	10.99	A341	0 0 0 0 0	
2.543E-01	2.851E+01	11.99	A341	0 0 0 0 0	
3.310E-01	3.710E+01	15	F300	1 0 0 0 2	
2.606E-01	2.921E+01	15.99	A341	0 0 0 0 0	
3.385E-01	3.794E+01	20.99	A341	0 0 0 0 0	
4.216E-01	4.725E+01	24.99	A341	0 0 0 0 0	
4.665E-01	5.229E+01	27.99	A341	0 0 0 0 0	
5.182E-01	5.808E+01	28.99	A341	0 0 0 0 0	
6.448E-01	7.227E+01	33.99	A341	0 0 0 0 0	
6.677E-01	7.484E+01	35.99	A341	0 0 0 0 0	
7.816E-01	8.761E+01	37.99	A341	0 0 0 0 0	
1.120E+00	1.256E+02	41.99	A341	0 0 0 0 0	
1.229E+00	1.378E+02	43.99	A341	0 0 0 0 0	
1.444E+00	1.618E+02	46.64	A341	0 0 0 0 0	
2.159E+00	2.420E+02	49.99	A341	0 0 0 0 0	
2.610E+00	2.926E+02	51.99	A341	0 0 0 0 0	
2.768E+00	3.103E+02	53.99	A341	0 0 0 0 0	
2.815E+00	3.155E+02	54.49	A341	0 0 0 0 0	
3.221E+00	3.610E+02	54.99	A341	0 0 0 0 0	
3.964E+00	4.443E+02	57.49	A341	0 0 0 0 0	
4.219E+00	4.729E+02	60.04	A341	0 0 0 0 0	
4.224E+00	4.735E+02	61.39	A341	0 0 0 0 0	
4.940E+00	5.537E+02	62.99	A341	0 0 0 0 0	
5.529E+00	6.197E+02	67.99	A341	0 0 0 0 0	
1.838E+00	2.060E+02	100	F300	1 0 0 0 2	

408. C₅H₄O₃

Isopyromucic acid

Isobrenzschleimsaeure

RN: 496-64-0 **MP (°C):**
MW: 112.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.845E-01	4.310E+01	0	F300	1 0 0 0 2	

409. C₅H₅Cl₃N₂OS

5-Ethoxy-3-trichloromethyl-1,2,4-thiadiazole

RN: 2593-15-9 **MP (°C):**
MW: 247.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.732E-04	1.171E-01	ns	S460	0 0 0 0 0	

410. C₅H₅NO

3-Hydroxypyridine

3-Pyridinol

RN: 109-00-2 **MP (°C):** 127.5
MW: 95.10 **BP (°C):** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.392E-01	3.226E+01	20	B050	1 0 0 0 0	

411. C₅H₅NO

4-Hydroxypyridine

4-Pyridinol

RN: 626-64-2 **MP (°C):** 148
MW: 95.10 **BP (°C):** 232.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.258E+00	5.000E+02	20	B050	1 0 0 0 0	

412. C₅H₅NO

2-Hydroxypyridine

2-Pyridinol

RN: 72762-00-6 **MP (°C):** 106
MW: 95.10 **BP (°C):** 280.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.258E+00	5.000E+02	20	B050	1 0 0 0 0	

413. C₅H₅NO₂

2,4-Dihydroxypyridine

3-Deazauracil

2,4-Pyridinediol

RN: 626-03-9 **MP (°C):** 278
MW: 111.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.591E-02	6.211E+00	20	B050	1 0 0 0 0	

414. C₅H₅N₃O

Pyrazinamide

Pyrazine-2-carboxamide

Prazina

RN: 98-96-4**MP (°C):** 190**MW:** 123.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-01	1.740E+01	25	N041	2 0 1 1 0	EFG
1.218E-01	1.500E+01	ns	K444	0 0 0 0 0	

415. C₅H₅N₅

Adenine

Adenin

6-Aminopurine

1H-Purin-6-amine

Adeninimine

Vitamin B4

RN: 73-24-5**MP (°C):** 363**MW:** 135.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.719E-03	6.377E-01	17.5	S306	1 0 1 2 2	
6.328E-03	8.551E-01	18.8	S306	1 0 1 2 2	
6.494E-03	8.776E-01	19.2	S306	1 0 1 2 2	
7.382E-03	9.975E-01	19.7	S306	1 0 1 2 2	
7.000E-03	9.459E-01	20	C017	2 0 0 1 0	EFG
6.907E-03	9.333E-01	20.08	D307	0 0 0 0 0	
7.680E-03	1.038E+00	22.36	D307	0 0 0 0 0	
6.586E-03	8.900E-01	25	A337	0 0 0 0 0	
7.200E-03	9.729E-01	25	C416	2 1 1 1 1	
5.476E-03	7.400E-01	25	C437	0 0 0 0 0	Average
6.654E-03	8.992E-01	25	D041	1 0 0 0 0	
7.040E-03	9.513E-01	25	H061	0 0 0 0 0	
7.600E-03	1.027E+00	25	L080	2 1 2 1 2	
8.000E-03	1.081E+00	25	R039	0 0 0 0 0	
8.610E-03	1.163E+00	25.01	D307	0 0 0 0 0	
8.690E-03	1.174E+00	25.03	D307	0 0 0 0 0	
8.250E-03	1.115E+00	25.5	T008	1 1 2 2 2	
7.936E-03	1.072E+00	26.6	S306	1 0 1 2 2	
9.740E-03	1.316E+00	27.47	D307	0 0 0 0 0	
1.087E-02	1.469E+00	29.97	D307	0 0 0 0 0	
9.377E-03	1.267E+00	31.1	S306	1 0 1 2 2	
1.540E-02	2.081E+00	37	L042	2 0 2 2 2	pH 6.47
1.390E-02	1.878E+00	38	T008	1 1 2 2 2	
1.514E-02	2.045E+00	44.0	S306	1 0 1 2 2	
1.707E-02	2.307E+00	45.1	S306	1 0 1 2 2	
1.862E-02	2.516E+00	45.5	S306	1 0 1 2 2	

(continued)

415. C₅H₅N₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.805E-01	2.439E+01	100	D041	1 0 0 0 0	
6.808E-03	9.200E-01	c	D004	0 0 0 0 0	
1.805E-01	2.439E+01	h	D004	0 0 0 0 0	

416. C₅H₅N₅O

Guanine

2-Aminohypoxanthine

2-Amino-6-hydroxypurine

RN: 73-40-5 MP (°C): >300
 MW: 151.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-05	2.902E-03	15.02	D307	0 0 0 0 0	
6.000E-05	9.068E-03	20	C017	2 0 0 1 1	EFG
2.740E-05	4.141E-03	20.05	D307	0 0 0 0 0	
3.290E-05	4.972E-03	22.50	D307	0 0 0 0 0	
3.870E-05	5.849E-03	25.02	D307	0 0 0 0 0	
4.520E-05	6.831E-03	27.54	D307	0 0 0 0 0	
5.350E-05	8.085E-03	30.01	D307	0 0 0 0 0	
7.230E-05	1.093E-02	35.05	D307	0 0 0 0 0	
2.647E-04	4.000E-02	40	D041	1 0 0 0 0	
9.880E-05	1.493E-02	40.22	D307	0 0 0 0 0	
3.311E-04	5.004E-02	ns	R424	0 0 0 0 0	
3.311E-04	5.004E-02	ns	R427	0 0 0 0 0	

417. C₅H₅N₅O

Isoguanine

2-Hydroxy-6-aminopurine

RN: 3373-53-3 MP (°C):
 MW: 151.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.970E-04	6.000E-02	25	D041	1 0 0 0 0	
1.654E-03	2.499E-01	100	D041	1 0 0 0 1	

418. C₅H₅N₅O₂

2,8-Dioxyadenine

2,8-Dihydroxyadenine

RN: 30377-37-8 MP (°C):
 MW: 167.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-05	2.200E-03	25	B049	1 0 1 1 1	
8.556E-06	1.430E-03	37	P068	0 0 0 0 0	

419. C₅H₆

Cyclopentadiene

Pentolex

Pentole

Pyropentylene

R-Pentine

1,3-Cyclopentadiene

RN: 542-92-7 **MP (°C):** -85**MW:** 66.10 **BP (°C):** 42

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.023E-02	6.764E-01	ns	S460	0 0 0 0 0	

420. C₅H₆Cl₂N₂

3-Methyluracil

2,4(1H,3H)-Pyrimidinedione, 3-methyl-

Uracil, 3-methyl-

RN: 608-34-4 **MP (°C):****MW:** 165.02 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.212E+00	2.000E+02	ns	B177	0 0 0 0 2	

421. C₅H₆Cl₂N₂O₂

Dantoin

1,3-Dichloro-5,5-dimethyl-2,4-imidazolidinedione

1,3-Dichloro-5,5-dimethylhydantoin

RN: 118-52-5 **MP (°C):** 132**MW:** 197.02 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.537E-03	4.998E-01	20	B080	1 0 1 1 0	
6.590E-03	1.298E+00	40	B080	1 0 1 1 1	

422. C₅H₆N₂OS

Methylthiouracil

6-Methyl-2-thiouracil

RN: 56-04-2 **MP (°C):** 330**MW:** 142.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-03	5.332E-01	25	G016	1 2 1 2 2	intrinsic
7.026E-03	9.990E-01	c	I310	0 0 0 0 0	
3.715E-03	5.283E-01	ns	R424	0 0 0 0 0	

423. C₅H₆N₂OS

5-Methyl-2-thiouracil

4(1H)-Pyrimidinone, 2,3-dihydro-5-methyl-2-thioxo-
2-Thiothymine**RN:** 636-26-0 **MP (°C):** 284**MW:** 142.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.580E-03	5.090E-01	25	G016	1 2 1 2 2	intrinsic

424. C₅H₆N₂O₂

Thymine

2,4-Dihydroxy-5-methylpyrimidine

5-Methyluracil

RN: 65-71-4 **MP (°C):** 316**MW:** 126.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-02	2.775E+00	20	C017	2 0 0 1 1	EFG
2.379E-02	3.000E+00	23	F300	1 0 0 0 0	
3.552E-02	4.480E+00	25	D041	1 0 0 0 1	
2.780E-02	3.506E+00	25	H061	0 0 0 0 0	
3.030E-02	3.821E+00	25	L080	2 1 2 1 2	
2.860E-02	3.607E+00	25	R039	0 0 0 0 0	
2.740E-02	3.456E+00	25.5	T008	1 1 2 2 2	
3.500E-02	4.414E+00	30	L080	2 1 2 1 2	

425. C₅H₆N₂O₂

1-Methyluracil

2,4(1H,3H)-Pyrimidinedione, 1-methyl-

N1-Methyluracil

RN: 615-77-0 **MP (°C):** 179**MW:** 126.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.586E-01	2.000E+01	ns	B177	0 0 0 0 1	

426. C₅H₆N₂O₄

5-Carboxymethylhydantoin

Hydantoin of aspartic acid

RN: 5427-26-9 **MP (°C):** 216**MW:** 158.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.050E-02	1.115E+01	ns	M025	0 2 0 1 2	

427. C₅H₆O₂

α -Angelica lactone
 α -Angelica-lacton

RN: 591-12-8 **MP (°C):** 18
MW: 98.10 **BP (°C):** 56

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.689E-01	4.600E+01	15	F300	1 0 0 0 1	

428. C₅H₆O₄

Citraconic acid
Citraconsaeure

RN: 498-23-7 **MP (°C):**
MW: 130.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.018E+00	7.830E+02	25	F300	1 0 0 0 2	

429. C₅H₆O₄

Mesaconic acid
Mesaconsaeure

RN: 498-24-8 **MP (°C):** 204.5
MW: 130.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.022E-01	2.630E+01	18	F300	1 0 0 0 2	
4.241E+00	5.518E+02	100	F300	1 0 0 0 2	

430. C₅H₆O₄

Itaconic acid
Itaconsaeure

RN: 97-65-4 **MP (°C):** 163
MW: 130.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.281E-01	5.570E+01	10	F300	1 0 0 0 2	
5.891E-01	7.664E+01	20	D041	1 0 0 0 1	
5.903E-01	7.680E+01	20	F300	1 0 0 0 2	

431. C₅H₆S

3-Methylthiophene

RN: 616-44-4

MP (°C): -69

MW: 98.17

BP (°C): 114 at 738 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-03	3.999E-01	ns	S460	0 0 0 0 0	

432. C₅H₇NO₂

Ethyl cyanoacetate

Cyanessigsaeure-aethyl ester

RN: 105-56-6

MP (°C):

MW: 113.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.768E-01	2.000E+01	25	F300	1 0 0 0 0	
7.072E-01	8.000E+01	80	F300	1 0 0 0 0	

433. C₅H₇NO₄S

2,4-Thiazolidinedicarboxylic acid

Tidiacic acid

Tidiacic

TDCA

RN: 30097-06-4

MP (°C):

MW: 177.18

BP (°C): 524.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-02	7.619E+00	21	B414	1 0 0 1 1	

434. C₅H₇N₂O₂

6-Methyluracil

4-Methyl-uracil

RN: 626-48-2

MP (°C): 318dec

MW: 127.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.506E-02	7.000E+00	22	F300	1 0 0 0 0	

435. C₅H₇N₃O

5-Methylcytosine

Mec

RN: 554-01-8

MP (°C): 270

MW: 125.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.441E-01	4.306E+01	25	D041	1 0 0 0 1	

436. C₅H₇N₃O₂

Dimetridazole

1,2-Dimethyl-5-nitroimidazole

RN: 551-92-8 **MP (°C):** 137–139
MW: 141.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.866E-02	9.690E+00	20	D344	0 0 0 0 0	
6.866E-02	9.690E+00	20	D344	0 0 0 0 0	
6.738E-02	9.509E+00	20	D344	0 0 0 0 0	
6.870E-02	9.696E+00	20	D344	0 0 0 0 0	

437. C₅H₈

Isoprene

2-Methyl-1,3-butadiene

RN: 78-79-5 **MP (°C):** -120
MW: 68.12 **BP (°C):** 34.07

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.425E-03	6.420E-01	25	M001	2 1 2 2 2	

438. C₅H₈

Cyclopentene

RN: 142-29-0 **MP (°C):** -135
MW: 68.12 **BP (°C):** 44

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.411E-02	1.642E+00	24.8	L007	2 1 1 2 2	
7.854E-03	5.350E-01	25	M001	2 1 2 2 2	
2.411E-02	1.642E+00	25.1	L007	2 2 1 1 2	
2.562E-02	1.745E+00	34.8	L007	2 1 1 2 2	

439. C₅H₈

1-Pentyne

Pent-1-yne

RN: 627-19-0 **MP (°C):** -106
MW: 68.12 **BP (°C):** 40

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.305E-02	1.570E+00	25	M001	2 1 2 2 2	
1.154E-02	7.861E-01	25	M342	1 0 1 1 2	

440. C₅H₈

1,4-Pentadiene

Penta-1,4-diene

RN: 591-93-5

MP (°C): -148

MW: 68.12

BP (°C): 26

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.191E-03	5.580E-01	25	M001	2 1 2 2 2	

441. C₅H₈BrNO₄

5-Bromo-2-methyl-5-nitro-1,3-dioxane

Dioxane, 5-bromo-2-methyl-5-nitro-

Nibroxane

RN: 53983-00-9 MP (°C): 72

MW: 226.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.695E-02	6.093E+00	25	L013	1 0 2 1 2	

442. C₅H₈N₂O₂

5,5'-Dimethylhydantoin

5,5-Dimethylhydantoin

5,5-Dimethyl-2,4-imidazolidinedione

5,5-Dimethylimidazolidine-2,4-dione

RN: 77-71-4 MP (°C): 177

MW: 128.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E+00	1.304E+02	37	F183	1 0 1 1 1	intrinsic

443. C₅H₈N₂O₂

5-Ethylhydantoin

Hydantoin of α -aminobutyric acid

RN: 15414-82-1 MP (°C): 119

MW: 128.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-01	1.106E+02	ns	M025	0 2 0 1 2	

444. C₅H₈N₄O₃S₂

Methazolamide

Acetamide, *N*-[5-(aminosulfonyl)-3-methyl-1,3,4-thiadiazol-2(3H)-ylidene]-
N-(4-Methyl-2-sulfamoyl-D2-1,3,4-thiadiazolin-5-ylidene)acetamide

Neptazaneat

Metazolamide

Methenamide

RN: 554-57-4 **MP (°C):** 213**MW:** 236.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	4.725E-01	15	K024	1 2 1 1 1	
1.200E-02	2.835E+00	25	C415	1 0 0 1 0	
2.963E-03	7.000E-01	amb	L434	0 0 0 0 0	
1.481E-02	3.500E+00	ns	M032	0 0 0 0 2	
1.479E-02	3.495E+00	ns	R428	0 0 0 0 0	

445. C₅H₈N₄O₁₂

Pentaerythritol tetranitrate

Nitropentaerythritol

1,3-Propanediol, 2,2-*bis*[(nitrooxy)methyl]-, dinitrate (ester)**RN:** 78-11-5 **MP (°C):** 140**MW:** 316.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.326E-06	2.000E-03	ns	M013	0 2 0 1 1	

446. C₅H₈O

Cyprethylene ether

RN: **MP (°C):****MW:** 84.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.435E-02	7.937E+00	27	K058	1 0 1 1 0	

447. C₅H₈O

α-Methylcrotonaldehyde

α-Methyl-crotonaldehyd

RN: 623-36-9 **MP (°C):****MW:** 84.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.378E-01	2.000E+01	20	F300	1 0 0 0 1	

448. C₅H₈O₂

Ethyl acrylate

Ethyl propenoate

2-Propenoic acid ethyl ester

RN: 140-88-5 **MP (°C):** -71
MW: 100.12 **BP (°C):** 99.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.785E-01	1.787E+01	30	L096	1 2 0 2 2	

449. C₅H₈O₂

Methyl methacrylate

Methacrylic acid methyl ester

Methyl 2-methyl-2-propenoate

RN: 80-62-6 **MP (°C):** -48
MW: 100.12 **BP (°C):** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.563E-01	1.565E+01	20	L096	1 2 0 2 2	

450. C₅H₈O₂

Acetylacetone

2,4-Pentanedione

Acetylacetone

RN: 123-54-6 **MP (°C):** -23
MW: 100.12 **BP (°C):** 140.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.678E+00	1.680E+02	19.0	N051	1 2 1 1 2	
1.703E+00	1.705E+02	19.5	N051	1 2 1 1 2	
1.089E+00	1.090E+02	20	F300	1 0 0 0 2	
1.706E+00	1.708E+02	25	B019	1 0 1 2 0	

451. C₅H₈O₃

Dimethylpyruvic acid

DL-Methyl-bernsteinsaeure

α-Ketoisovaleric acid

RN: 759-05-7 **MP (°C):**
MW: 116.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E+00	4.006E+02	20	F300	1 0 0 0 2	

452. C₅H₈O₃

Levulinic acid

Laevulinsaeure

4-Oxopentanoic acid

3-Acetyl propionic acid

RN: 123-76-2 MP (°C): 37.2

MW: 116.12 BP (°C): 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.632E+00	5.378E+02	6.99	A340	0 0 0 0 0	
4.990E+00	5.795E+02	9.99	A340	0 0 0 0 0	
5.530E+00	6.422E+02	14.49	A340	0 0 0 0 0	
6.087E+00	7.068E+02	20.79	A340	0 0 0 0 0	
6.400E+00	7.431E+02	24.99	A340	0 0 0 0 0	
6.631E+00	7.700E+02	30.09	A340	0 0 0 0 0	

453. C₅H₈O₄

Methylsuccinic acid

Acide methylsuccinique

1,2-Propanedicarboxylic acid

RN: 498-21-5 MP (°C): 117.5

MW: 132.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.041E+00	6.660E+02	15	M051	1 0 0 0 2	

454. C₅H₈O₄

Ethylmalonic acid

1,1-Propanedicarboxylic acid

Aethylmalonsaeure

Mono-ethyl malonate

Malonic acid monoethyl ester

Malonsaeure-monoethyl ester

RN: 601-75-2 MP (°C): 114

MW: 132.12 BP (°C): 160

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.619E+00	3.460E+02	0	F300	1 0 0 0 2	
3.996E+00	5.280E+02	0	M051	1 0 0 0 2	
4.814E+00	6.360E+02	15	M051	1 0 0 0 2	
5.389E+00	7.120E+02	25	M051	1 0 0 0 2	
3.626E+00	4.790E+02	50	F300	1 0 0 0 2	
6.873E+00	9.080E+02	50	M051	1 0 0 0 2	

455. C₅H₈O₄

Dimethylmalonic acid

Dimethyl-malonsaeure

Dimethyl-propanedioic acid

RN: 595-46-0 MP (°C): 192

MW: 132.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.812E-01	9.000E+01	13	F300	1 0 0 0 0	
1.968E+00	2.600E+02	100	F300	1 0 0 0 1	

456. C₅H₈O₄

Glutaric acid

Glutarsaeure

1,3-Propanedicarboxylic acid

RN: 110-94-1 MP (°C): 96.5

MW: 132.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.272E+00	3.002E+02	0	F300	1 0 0 0 2	
3.247E+00	4.290E+02	0	L041	1 0 0 1 2	
2.410E+00	3.183E+02	3.40	A031	1 2 2 2 2	
2.650E+00	3.501E+02	5.99	A341	0 0 0 0 0	
2.764E+00	3.651E+02	7.99	A341	0 0 0 0 0	
3.127E+00	4.131E+02	10.40	A031	1 2 2 2 2	
2.909E+00	3.843E+02	10.99	A341	0 0 0 0 0	
3.213E+00	4.245E+02	12.99	A341	0 0 0 0 0	
3.433E+00	4.536E+02	14	A031	1 2 2 2 0	
4.443E+00	5.870E+02	15	L041	1 0 0 1 2	
4.443E+00	5.870E+02	15	M051	1 0 0 0 2	
3.521E+00	4.652E+02	15.99	A341	0 0 0 0 0	
3.674E+00	4.854E+02	17.99	A341	0 0 0 0 0	
3.861E+00	5.100E+02	18	A031	1 2 2 2 2	
3.816E+00	5.041E+02	19.99	A341	0 0 0 0 0	
2.954E+00	3.902E+02	20	D041	1 0 0 0 1	
4.837E+00	6.390E+02	20	L041	1 0 0 1 2	
2.952E+00	3.900E+02	20	M171	1 0 0 0 2	
1.340E+00	1.770E+02	20	S006	1 0 0 0 2	
4.278E+00	5.652E+02	23.90	A031	1 2 2 2 2	
4.088E+00	5.401E+02	24.99	A341	0 0 0 0 0	
4.653E+00	6.148E+02	28.30	A031	1 2 2 2 2	
4.394E+00	5.805E+02	28.99	A341	0 0 0 0 0	
4.503E+00	5.949E+02	30.99	A341	0 0 0 0 0	
4.642E+00	6.133E+02	33.99	A341	0 0 0 0 0	
6.033E+00	7.970E+02	35	L041	1 0 0 1 2	
4.796E+00	6.336E+02	36.99	A341	0 0 0 0 0	
4.894E+00	6.466E+02	38.99	A341	0 0 0 0 0	
5.096E+00	6.732E+02	42.99	A341	0 0 0 0 0	
5.131E+00	6.779E+02	43.99	A341	0 0 0 0 0	
5.143E+00	6.795E+02	44.99	A341	0 0 0 0 0	

(continued)

456. C₅H₈O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.246E+00	6.930E+02	46.99	A341	0 0 0 0 0	
5.341E+00	7.057E+02	49.99	A341	0 0 0 0 0	
7.244E+00	9.570E+02	50	L041	1 0 0 1 2	
5.470E+00	7.227E+02	54.49	A341	0 0 0 0 0	
5.640E+00	7.451E+02	55.99	A341	0 0 0 0 0	
5.713E+00	7.548E+02	58.99	A341	0 0 0 0 0	
5.729E+00	7.569E+02	61.09	A341	0 0 0 0 0	
5.890E+00	7.782E+02	62.99	A341	0 0 0 0 0	
4.032E+00	5.327E+02	65	F300	1 0 0 0 2	
8.462E+00	1.118E+03	65	L041	1 0 0 1 2	
6.038E+00	7.977E+02	68.99	A341	0 0 0 0 0	
4.081E+00	5.392E+02	rt	H431	0 0 0 0 0	

457. C₅H₉BrO₂ α -Bromo-methyl-ethyl-acetateEthyl DL- α -bromopropionate

Propanoic acid, 2-bromo-, ethyl ester

Ethyl DL-2-bromopropionate

RN: 535-11-5 MP (°C):

MW: 181.04 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E-01	5.033E+01	ns	F057	0 2 2 2 1	

458. C₅H₉BrO₂ α -Ethyl- β -bromo-propionic ureide

RN: MP (°C):

MW: 181.04 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.130E-01	3.855E+01	ns	F056	0 2 2 2 1	

459. C₅H₉NO₂

DL-Proline

Pyrrolidine-2-carboxylic acid

RN: 609-36-9 MP (°C): 208

MW: 115.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.217E+01	1.401E+03	20	J303	0 0 0 0 0	
1.146E+01	1.319E+03	25	J303	0 0 0 0 0	
1.425E+01	1.641E+03	40	J303	0 0 0 0 0	
1.708E+01	1.967E+03	50	J303	0 0 0 0 0	
2.082E+01	2.397E+03	60	J303	0 0 0 0 0	

460. C₅H₉NO₂

L-Proline

2-Pyrrolidinecarboxylic acid

RN: 147-85-3 **MP (°C):**
MW: 115.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.374E+00	6.188E+02	25	D041	1 0 0 0 2	
6.653E+00	7.660E+02	27	D036	0 0 0 0 0	
6.123E+00	7.050E+02	65	D041	1 0 0 0 2	
6.691E+00	7.704E+02	99.99	P349	0 0 0 0 0	

461. C₅H₉NO₂S

2-Methylthiazolidine-4-carboxylic acid

4-Thiazolidinecarboxylic acid, 2-methyl-
Thiazolidine-4-carboxylic acid, 2-methyl-

RN: 4165-32-6 **MP (°C):** 174-175
MW: 147.20 **BP (°C):** 333.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-01	3.091E+01	21	B414	1 0 0 1 1	partial decomposition

462. C₅H₉NO₃

L-Hydroxyproline

trans-4-Hydroxy-L-proline

L-4-hydroxyproline

(4S)-4-Hydroxy-L-proline

RN: 51-35-4 **MP (°C):**
MW: 131.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.158E+00	4.141E+02	99.99	P349	0 0 0 0 0	

463. C₅H₉NO₃Formyl- α -aminobutyric acid

Butanoic acid, 2-(formylamino)-

RN: 106873-99-8 **MP (°C):**
MW: 131.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-01	3.357E+01	25	M024	1 2 0 1 2	
2.560E-01	3.357E+01	ns	M025	0 2 0 1 2	

464. C₅H₉NO₄

D-Glutamic acid

D-2-Aminoglutamic acid

RN: 6893-26-1 **MP (°C):** 201
MW: 147.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.337E-02	3.439E+00	0	D018	2 2 2 1 2	
2.303E-02	3.388E+00	0	M043	1 0 0 0 1	
3.381E-02	4.975E+00	10	M043	1 0 0 0 1	
1.004E-01	1.478E+01	20	D041	1 0 0 0 1	
4.859E-02	7.149E+00	20	M043	1 0 0 0 1	
4.472E-02	6.580E+00	21	P045	1 0 2 1 2	
5.981E-02	8.800E+00	25	D018	2 2 2 1 2	
6.729E-02	9.901E+00	30	M043	1 0 0 0 1	
1.004E-01	1.478E+01	40	M043	1 0 0 0 1	
1.481E-01	2.179E+01	50	D018	2 2 2 1 2	
2.107E-01	3.101E+01	60	M043	1 0 0 0 1	
4.148E-01	6.103E+01	80	M043	1 0 0 0 1	
8.347E-01	1.228E+02	100	M043	1 0 0 0 2	
5.850E-02	8.607E+00	ns	M025	0 2 0 1 2	

465. C₅H₉NO₄

DL-Glutamic acid

DL-2-Aminoglutamic acid

RN: 617-65-2 **MP (°C):** 194
MW: 147.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.601E-02	8.241E+00	0	D018	2 2 2 1 2	
4.850E-02	7.136E+00	4.99	A405	2 0 1 1 2	
5.990E-02	8.813E+00	9.99	A405	2 0 1 1 2	
6.300E-02	9.269E+00	14.99	A405	2 0 1 1 2	
8.840E-02	1.301E+01	20.99	A405	2 0 1 1 2	
9.370E-02	1.379E+01	24.99	A405	2 0 1 1 2	
1.750E-01	2.575E+01	25	D018	2 2 2 1 2	
1.368E-01	2.013E+01	25	D041	1 0 0 0 2	
1.075E-01	1.582E+01	29.99	A405	2 0 1 1 2	
1.414E-01	2.080E+01	34.99	A405	2 0 1 1 2	
1.684E-01	2.478E+01	39.99	A405	2 0 1 1 2	
2.016E-01	2.966E+01	44.99	A405	2 0 1 1 2	
2.699E-01	3.971E+01	49.99	A405	2 0 1 1 2	
5.131E-01	7.549E+01	50	D018	2 2 2 1 2	
3.502E-01	5.153E+01	54.99	A405	2 0 1 1 2	
3.959E-01	5.825E+01	59.99	A405	2 0 1 1 2	
4.772E-01	7.021E+01	64.99	A405	2 0 1 1 2	
5.621E-01	8.270E+01	69.99	A405	2 0 1 1 2	
6.709E-01	9.871E+01	71.99	A405	2 0 1 1 2	
7.289E-01	1.072E+02	74.99	A405	2 0 1 1 2	
7.206E-01	1.060E+02	75	D041	1 0 0 0 2	

466. C₅H₉NO₄

L-Glutamic acid

L-2-Aminoglutamic acid

L(+)-Glutaminsaeure

Glutamic acid

L(+) Glutaminic acid

RN: 56-86-0**MP (°C):** 250**MW:** 147.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.866E-02	7.160E+00	20	B032	1 2 2 1 2	
4.486E-02	6.600E+00	21	F302	1 0 0 0 1	
5.825E-02	8.570E+00	25	B032	1 2 2 1 2	
5.822E-02	8.566E+00	25	D041	1 0 0 0 2	
5.845E-02	8.600E+00	25	F300	1 0 0 0 1	
7.262E-02	1.068E+01	25	G315	0 0 0 0 0	
5.614E-02	8.260E+00	27	D036	0 0 0 0 0	
6.980E-02	1.027E+01	29.80	B032	1 2 2 1 2	
1.454E-01	2.140E+01	50	F300	1 0 0 0 2	
3.562E-01	5.240E+01	75	D041	1 0 0 0 2	
3.561E-01	5.240E+01	75	F300	1 0 0 0 2	
8.346E-01	1.228E+02	100	F300	1 0 0 0 2	
4.078E-02	6.000E+00	ns	D072	0 0 0 0 0	
5.802E-02	8.537E+00	rt	H431	0 0 0 0 0	

467. C₅H₁₀

Cyclopentane

Pentamethylene

Exxsol cyclopentane S

Zeonsolv HP

RN: 287-92-3**MP (°C):** -94.4**MW:** 70.14**BP (°C):** 49.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.826E-03	3.385E-01	4.8	L007	2 2 1 2 2	
4.826E-03	3.385E-01	5.1	L007	2 1 1 1 2	
4.870E-03	3.416E-01	14.8	L007	2 2 1 2 2	
4.870E-03	3.416E-01	15.2	L007	2 1 1 1 2	
4.873E-03	3.418E-01	24.8	L007	2 2 1 2 2	
2.338E-03	1.640E-01	25	G313	2 1 1 2 2	
2.281E-03	1.600E-01	25	K119	1 0 0 0 2	
2.224E-03	1.560E-01	25	M001	2 1 2 2 2	
2.224E-03	1.560E-01	25	M002	2 1 2 2 2	
2.281E-03	1.600E-01	25.0	P051	2 1 1 2 2	
2.281E-03	1.600E-01	25.00	P007	2 1 2 2 2	
4.873E-03	3.418E-01	25.1	L007	2 1 1 1 2	
5.252E-03	3.684E-01	34.8	L007	2 2 1 2 2	
5.252E-03	3.684E-01	35.2	L007	2 1 1 1 2	
2.324E-03	1.630E-01	40.1	P051	2 1 1 2 2	

(continued)

467. C₅H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.324E-03	1.630E-01	40.10	P007	2 1 2 2 2	
4.867E-03	3.414E-01	44.8	L007	2 2 1 2 2	
2.566E-03	1.800E-01	55.7	P051	2 1 1 2 2	
2.566E-03	1.800E-01	55.70	P007	2 1 2 2 2	
4.220E-03	2.960E-01	99.1	P051	2 1 1 2 2	
4.220E-03	2.960E-01	99.10	P007	2 1 2 2 2	
5.304E-03	3.720E-01	118.0	P051	2 1 1 2 2	
5.304E-03	3.720E-01	118.00	P007	2 1 2 2 2	
8.712E-03	6.110E-01	137.3	P051	2 1 1 2 2	
8.712E-03	6.110E-01	137.30	P007	2 1 2 2 2	
1.129E-02	7.920E-01	153.1	P051	2 1 1 2 2	
1.129E-02	7.920E-01	153.10	P007	2 1 2 2 2	
2.224E-03	1.560E-01	ns	H123	0 0 0 0 0	

468. C₅H₁₀

3-Methyl-1-butene

2-Methyl-3-butene

3,3-Dimethylpropene

Isopropylethylene

RN: 563-45-1 MP (°C): -168

MW: 70.14 BP (°C): 20

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-03	1.300E-01	25	M001	2 1 2 2 2	

469. C₅H₁₀

2-Pentene

1-Methyl-2-ethylethylene

sym-Methylethylethylene

β-Amylene

β-n-Amylene

3-Pentene

RN: 109-68-2 MP (°C): -136

MW: 70.14 BP (°C): 36

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.894E-03	2.030E-01	25	M001	2 1 2 2 2	

470. C₅H₁₀

1-Pentene

Propylethylene

 α -n-Amylene

1-Methyl-3-butene

RN: 109-67-1

MP (°C): -165

MW: 70.14

BP (°C): 30.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.609E-03	1.830E-01	23	C332	0 0 0 0 0	
2.110E-03	1.480E-01	25	M001	2 1 2 2 2	

471. C₅H₁₀Cl₃O₃P

Diethyl trichloromethyl phosphonate

Phosphonic acid, (trichloromethyl)-, diethyl ester

Ro 3-0658

RN: 866-23-9

MP (°C):

MW: 255.47

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.761E-02	4.500E+00	25	B070	1 2 0 1 1	

472. C₅H₁₀N₂O

N-Nitrosopiperidine

Pyridine, hexahydro-*N*-nitroso

NPIP

RN: 100-75-4

MP (°C): <25

MW: 114.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-01	7.648E+01	24	D083	2 0 0 0 1	

473. C₅H₁₀N₂O₂S

Methomyl

Nudrin

Lannate

RN: 16752-77-5

MP (°C): 78.5

MW: 162.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.576E-01	5.800E+01	25	M161	1 0 0 0 1	

474. C₅H₁₀N₂O₃

Glycolylglycineamide

RN:

MP (°C):

MW: 146.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.820E+00	8.506E+02	25	M008	1 0 0 0 2	

475. C₅H₁₀N₂O₃

Glycyl-L-alanine

Glycylalanine

RN: 3695-73-6

MP (°C):

MW: 146.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E+00	6.986E+02	24.99	B441	0 0 0 0 0	

476. C₅H₁₀N₂O₃

D-Glutamine

D-2-Aminoglutaramic acid

RN: 5959-95-5

MP (°C):

MW: 146.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.910E-01	4.253E+01	ns	M025	0 2 0 1 2	

477. C₅H₁₀N₂O₃

L-Glutamine

L(+)-Glutamin

L(+)-Glutamine

Glutamine

RN: 56-85-9

MP (°C): 185

MW: 146.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.184E-01	1.730E+01	0	F300	1 0 0 0 2	
2.378E-01	3.475E+01	18	D041	1 0 0 0 1	
2.444E-01	3.572E+01	20	B032	1 2 2 1 2	
2.829E-01	4.135E+01	25	B032	1 2 2 1 2	
2.789E-01	4.077E+01	25	D041	1 0 0 0 2	
2.701E-01	3.948E+01	25	G315	0 0 0 0 0	
5.891E-02	8.610E+00	25	J303	0 0 0 0 0	
2.997E-01	4.380E+01	25.1	N024	0 0 0 0 0	
2.840E-01	4.150E+01	25.1	N025	0 0 0 0 0	
2.840E-01	4.150E+01	25.1	N026	0 0 0 0 0	

(continued)

477. C₅H₁₀N₂O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.821E-01	4.123E+01	25.1	N027	1 1 2 2 2	
2.737E-01	4.000E+01	27	D036	0 0 0 0 0	
3.285E-01	4.801E+01	29.80	B032	1 2 2 1 2	
3.154E-01	4.610E+01	30	F300	1 0 0 0 2	
1.002E-01	1.464E+01	40	J303	0 0 0 0 0	
2.135E-01	3.120E+01	60	J303	0 0 0 0 0	

478. C₅H₁₀N₂S₂

Dazomet

3,5-Dimethyl-1,2,3,5-tetrahydro-1,3,5-thiadiazinethione-2

Thiazone

Thiazone

RN: 533-74-4 MP (°C): 106.5

MW: 162.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.386E-03	1.199E+00	25	M061	1 0 0 0 1	
1.169E-02	1.896E+00	30	B185	0 0 0 0 0	
7.395E-03	1.200E+00	30	M161	1 0 0 0 1	

479. C₅H₁₀N₆O₂

Dinitrosopentamethylenetetramine

3,7-Dinitroso-1,3,5,7-tetraazabicyclo[3.3.1]nonane

RN: 101-25-7 MP (°C): 207

MW: 186.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.318E-02	9.901E+00	ns	I313	0 0 0 0 0	

480. C₅H₁₀O

Methyl propyl ketone

Methyl propyl ketone

2-Pentanone

Pantan-2-one

RN: 107-87-9 MP (°C): -78

MW: 86.13 BP (°C): 100.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.870E-01	7.640E+01	10	G032	1 2 1 1 2	
6.520E-01	5.616E+01	20	G030	1 2 0 0 2	
5.000E-01	4.307E+01	20	M312	1 0 0 0 1	
6.799E-01	5.857E+01	25	A356	0 0 0 0 0	
4.786E-01	4.123E+01	25	B060	2 0 1 1 1	

(continued)

480. C₅H₁₀O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.775E-01	6.697E+01	25	C333	0 0 0 0 0	
7.000E-01	6.029E+01	25	F044	1 0 0 0 1	
6.063E-01	5.222E+01	25	G030	1 2 0 0 2	
6.572E-01	5.660E+01	25	P055	1 0 0 0 2	
5.718E-01	4.925E+01	30	G030	1 2 0 0 2	
6.300E-01	5.426E+01	30	G032	1 2 1 1 2	
5.806E-01	5.001E+01	35	A356	0 0 0 0 0	
6.799E-01	5.857E+01	35	C333	0 0 0 0 0	
5.302E-01	4.567E+01	45	A356	0 0 0 0 0	
6.799E-01	5.857E+01	45	C333	0 0 0 0 0	
5.150E-01	4.436E+01	50	G032	1 2 1 1 2	
5.302E-01	4.567E+01	55	A356	0 0 0 0 0	
5.806E-01	5.001E+01	55	C333	0 0 0 0 0	

481. C₅H₁₀O

Valeraldehyde

n-Valeraldehyde

Valeral

n-Pentanal

RN: 110-62-3 **MP (°C):** -92
MW: 86.13 **BP (°C):** 103

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.358E-01	1.170E+01	25	A049	1 0 0 0 2	
2.100E-01	1.809E+01	25	K012	1 0 0 0 1	

482. C₅H₁₀O

Tetrahydropyran

Pentamethylene oxide

RN: 142-68-7 **MP (°C):** -49.2
MW: 86.13 **BP (°C):** 88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.372E+00	1.182E+02	0	B001	2 0 1 0 0	
1.122E+00	9.666E+01	10	B001	2 0 1 0 0	
1.021E+00	8.792E+01	15	B001	2 0 1 0 0	
9.351E-01	8.054E+01	20	B001	2 0 1 0 0	
8.620E-01	7.425E+01	25	B001	2 0 1 0 0	

483. C₅H₁₀O

Diethyl ketone

3-Pentanone

RN: 96-22-0

MP (°C): -42

MW: 86.13

BP (°C): 101.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.810E-01	6.727E+01	10	G032	1 2 1 1 2	
4.786E-01	4.123E+01	20	D052	1 1 0 0 1	
5.613E-01	4.834E+01	20	G030	1 2 0 0 2	
6.052E-01	5.213E+01	25	B019	1 0 1 2 0	
3.818E-01	3.288E+01	25	B060	2 0 1 1 1	
5.328E-01	4.589E+01	25	G030	1 2 0 0 2	
5.900E-01	5.082E+01	25	K012	1 0 0 0 1	
4.999E-01	4.306E+01	30	G030	1 2 0 0 1	
5.760E-01	4.961E+01	30	G032	1 2 1 1 2	
4.560E-01	3.928E+01	50	G032	1 2 1 1 2	

484. C₅H₁₀O

1-Penten-3-ol

Penten-1-ol-3

RN: 616-25-1

MP (°C):

MW: 86.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.312E-01	8.021E+01	20	G031	1 0 0 0 2	
8.798E-01	7.579E+01	25	G031	1 0 0 0 2	
8.340E-01	7.184E+01	30	G031	1 0 0 0 2	

485. C₅H₁₀O

4-Penten-1-ol

Penten-4-ol-1

RN: 821-09-0

MP (°C):

MW: 86.13

BP (°C): 135.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.458E-01	5.562E+01	20	G031	1 0 0 0 2	
6.261E-01	5.393E+01	25	G031	1 0 0 0 2	
6.115E-01	5.267E+01	30	G031	1 0 0 0 2	

486. C₅H₁₀O

3-Penten-2-ol

Penten-3-ol-2

RN: 1569-50-2

MP (°C):

MW: 86.13

BP (°C): 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E+00	8.642E+01	20	G031	1 0 0 0 2	
9.508E-01	8.189E+01	25	G031	1 0 0 0 2	
9.075E-01	7.817E+01	30	G031	1 0 0 0 2	

487. C₅H₁₀O

2-Methyl tetrahydrofuran

2-Methyl oxolane

β-Methyl tetramethylene oxide

RN: 96-47-9

MP (°C): -136

MW: 86.13

BP (°C): 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.174E+00	1.011E+02	10	B001	2 0 1 0 0	

488. C₅H₁₀O

1-Methyl tetrahydrofuran

Methyl oxolane

α-Methyl tetramethylene oxide

RN: 45376-90-7

MP (°C):

MW: 86.13

BP (°C): 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.101E+00	1.810E+02	0	B001	2 0 1 0 0	
1.788E+00	1.540E+02	10	B001	2 0 1 0 0	
1.646E+00	1.418E+02	15	B001	2 0 1 0 0	
1.519E+00	1.308E+02	20	B001	2 0 1 0 0	
1.414E+00	1.218E+02	25	B001	2 0 1 0 0	

489. C₅H₁₀O

Cypreth ether

Cyclopropane, ethoxy-

Ethoxycyclopropane

Ethyl cyclopropyl ether

RN: 5614-38-0

MP (°C):

MW: 86.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-01	2.724E+01	25	K061	1 0 1 1 1	
2.500E-01	2.153E+01	25	K061	1 0 1 1 1	

490. C₅H₁₀O

3-Methyl-2-butanone

3-Methylbutanone-2

RN: 563-80-4 **MP (°C):** -92
MW: 86.13 **BP (°C):** 94.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.130E-01	7.003E+01	10	G032	1 2 1 1 2	
7.116E-01	6.130E+01	20	G030	1 2 0 0 2	
6.654E-01	5.732E+01	25	G030	1 2 0 0 2	
6.240E-01	5.375E+01	30	G030	1 2 0 0 2	
6.080E-01	5.237E+01	30	G032	1 2 1 1 2	
5.940E-01	5.116E+01	50	G032	1 2 1 1 2	

491. C₅H₁₀OS₂

Butylxanthogenic acid

RN: **MP (°C):**
MW: 150.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-04	1.202E-01	25	K012	1 0 0 0 0	

492. C₅H₁₀O₂

Valeric acid

Valeric acid, normal

n-Valeric acid

RN: 109-52-4 **MP (°C):** -34.5
MW: 102.13 **BP (°C):** 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.295E-01	2.344E+01	25	B060	2 0 1 1 1	
4.636E-01	4.735E+01	25	H028	2 0 2 0 2	
3.697E-01	3.776E+01	25	H122	1 0 0 0 2	
4.055E-01	4.141E+01	25	H338	2 2 1 2 2	
3.750E-01	3.830E+01	25	K012	1 0 0 0 2	
4.893E-01	4.997E+01	35	H338	2 2 1 2 2	
2.936E-03	2.999E-01	c	L055	0 0 0 0 1	
4.636E-01	4.735E+01	ns	A406	0 0 0 0 1	

493. C₅H₁₀O₂

Methyl butyrate

Buttersaeure-methyl ester

n-Methyl *n*-butyrate

RN: 623-42-7 **MP (°C):** -95
MW: 102.13 **BP (°C):** 102

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-01	1.561E+01	21	F001	1 0 1 2 2	
1.506E-01	1.538E+01	21	F300	1 0 0 0 2	
1.600E-01	1.634E+01	21	S006	1 0 0 0 2	
1.469E-01	1.500E+01	25	A049	1 0 0 0 2	

494. C₅H₁₀O₂

3-Hydroxy-2-methyltetrahydrofuran

3-Furanol, tetrahydro-2-methyl-

RN: 29848-44-0 **MP (°C):**
MW: 102.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.632E+00	1.667E+02	rt	B066	0 2 0 0 1	
4.896E+00	5.000E+02	rt	B066	0 2 0 0 2	

495. C₅H₁₀O₂

Propyl acetate

Essigsaeurepropyl ester

RN: 109-60-4 **MP (°C):** -92
MW: 102.13 **BP (°C):** 101.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-01	2.270E+01	20	E002	1 0 0 0 2	
1.850E-01	1.889E+01	20	F001	1 0 1 0 2	
1.821E-01	1.860E+01	20	F300	1 0 0 0 2	
1.800E-01	1.838E+01	20	M171	1 0 0 0 1	
2.220E-01	2.267E+01	21	S006	1 0 0 0 2	
1.920E-01	1.961E+01	25	B060	2 0 1 1 1	
1.731E-01	1.768E+01	30	R318	1 2 0 1 1	
1.960E-01	2.002E+01	37	E028	1 0 1 1 2	

496. C₅H₁₀O₂

Pivalic acid

Trimethylacetic acid

Trimethylessigsaeure

RN: 75-98-9 **MP (°C):** 35.5
MW: 102.13 **BP (°C):** 163.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.125E-01	2.170E+01	20	F300	1 0 0 0 2	

497. C₅H₁₀O₂

Isopropyl acetate

Essigsaeureisopropyl ester

Iso-propylacetat

RN: 108-21-4 **MP (°C):** -73
MW: 102.13 **BP (°C):** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-01	2.610E+01	20	D052	1 1 0 0 2	average of 2
3.030E-01	3.095E+01	20	F001	1 0 1 2 2	
2.937E-01	3.000E+01	20	F300	1 0 0 0 2	
2.108E-01	2.153E+01	24.6	H121	2 0 0 0 1	
2.759E-01	2.818E+01	25	B060	2 0 1 1 1	
1.930E-01	1.971E+01	37	E028	1 0 1 1 2	

498. C₅H₁₀O₂

Butyl formate

Formic acid butyl ester

RN: 592-84-7 **MP (°C):**
MW: 102.13 **BP (°C):** 106.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-02	1.001E+01	22	S006	1 0 0 0 1	
6.400E-02	6.537E+00	25	K012	1 0 0 0 1	
7.400E-02	7.558E+00	27	B052	1 0 1 1 2	
7.500E-02	7.660E+00	30.5	N014	0 0 0 0 0	
8.100E-02	8.273E+00	40.0	N014	0 0 0 0 0	

499. C₅H₁₀O₂

Ethyl propionate

Propanoic acid ethyl ester

RN: 105-37-3 MP (°C): -73
 MW: 102.13 BP (°C): 99

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.844E-01	1.884E+01	20	D052	1 1 0 0 2	
2.200E-01	2.247E+01	20	S006	1 0 0 0 1	
2.154E-01	2.200E+01	25	F300	1 0 0 0 1	
1.700E-01	1.736E+01	25	K012	1 0 0 0 1	
2.108E-01	2.153E+01	30	R318	1 1 0 1 1	

500. C₅H₁₀O₂

Isovaleric acid

Isovaleriansaeure

RN: 503-74-2 MP (°C): -29.3
 MW: 102.13 BP (°C): 176.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.946E-01	4.031E+01	20	D041	1 0 0 0 1	
3.985E-01	4.070E+01	20	F300	1 0 0 0 2	

501. C₅H₁₀O₃

Methyl β-methoxypropionate

Propionic acid, 3-methoxy-, methyl ester

Methyl 3-methoxypropanoate

Methyl 3-methoxypropionate

RN: 3852-09-3 MP (°C):
 MW: 118.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.628E+00	4.286E+02	25	R034	1 0 0 0 1	

502. C₅H₁₀O₃

Ethyl carbonate

Diethyl carbonate

RN: 105-58-8 MP (°C): -43
 MW: 118.13 BP (°C): 126

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.562E-01	1.845E+01	20	D052	1 1 0 0 2	

503. C₅H₁₀O₅

D-Xylose

 α -Xylose

Wood sugar

RN: 58-86-6**MP (°C):** 144.5**MW:** 150.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.879E+00	4.322E+02	25	G317	0 0 0 0 0	

504. C₅H₁₀O₅

L-Arabinose

L-Arabinopyranose

RN: 87-72-9**MP (°C):** 158**MW:** 150.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.482E+00	3.726E+02	10	F300	1 0 0 0 2	

505. C₅H₁₁Br

n-Amyl bromide

1-Bromopentane

Pentyl bromide

Amylene bromide

RN: 110-53-2**MP (°C):** -87.9**MW:** 151.05**BP (°C):** 129.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.380E-04	1.266E-01	25	M342	1 0 1 1 2	
1.800E-02	2.719E+00	ns	H307	0 0 0 0 0	

506. C₅H₁₁Br

Isoamyl bromide

1-Bromo-3-methylbutane

RN: 107-82-4**MP (°C):** -112**MW:** 151.05**BP (°C):** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.324E-03	2.000E-01	16	F300	1 0 0 0 1	
1.300E-03	1.964E-01	16.5	F001	1 0 1 0 2	

507. C₅H₁₁NO

Pentanamide

Valeramide

RN: 626-97-1 **MP (°C):** 102–104
MW: 101.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.530E-01	5.594E+01	6	H059	0 0 0 0 0	
6.360E-01	6.433E+01	16	H059	0 0 0 0 0	
7.880E-01	7.971E+01	25	H059	0 0 0 0 0	
1.108E+00	1.121E+02	37	H059	0 0 0 0 0	

508. C₅H₁₁NO₂

DL-Valine

DL-Valin

RN: 516-06-3 **MP (°C):** 296
MW: 117.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.593E-01	6.552E+01	0	D018	2 2 2 1 2	
5.711E-01	6.690E+01	25	C018	0 0 0 0 0	
6.035E-01	7.070E+01	25	D016	1 0 0 0 2	
5.912E-01	6.926E+01	25	D018	2 2 2 1 2	
5.614E-01	6.577E+01	25	D041	1 0 0 0 2	
5.975E-01	7.000E+01	25	F300	1 0 0 0 0	
7.352E-01	8.612E+01	50	D018	2 2 2 1 2	
7.170E-01	8.400E+01	50	F300	1 0 0 0 1	
1.003E+00	1.175E+02	75	D018	2 2 2 1 2	
9.559E-01	1.120E+02	75	D041	1 0 0 0 2	
9.560E-01	1.120E+02	75	F300	1 0 0 0 2	
1.349E+00	1.580E+02	100	F300	1 0 0 0 2	
1.351E+00	1.583E+02	99.99	P349	0 0 0 0 0	

509. C₅H₁₁NO₂

L-Norvaline

L-(+)-2-Aminovaleric acid

RN: 6600-40-4 **MP (°C):** >300
MW: 117.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.286E-01	9.707E+01	15	D041	1 0 0 0 2	

510. C₅H₁₁NO₂*tert*-Butyl carbamate*O-t*-Butyl carbamate

RN: 4248-19-5

MP (°C): 105

MW: 117.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.250E+00	1.464E+02	37	H006	1 2 2 1 2	
1.259E+00	1.475E+02	ns	R424	0 0 0 0 0	

511. C₅H₁₁NO₂*n*-Butyl carbamate

Butyl carbamate

RN: 592-35-8

MP (°C): 51

MW: 117.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-01	2.577E+01	37	H006	1 2 2 1 1	

512. C₅H₁₁NO₂

Isobutyl carbamate

iso-Butyl carbamate

RN: 543-28-2

MP (°C): 67

MW: 117.15

BP (°C): 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-01	5.857E+01	37	H006	1 2 2 1 0	

513. C₅H₁₁NO₂

DL-Isovaline

DL-Isovalin

RN: 595-39-1

MP (°C): 315

MW: 117.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.398E+00	2.809E+02	20	F300	1 0 0 0 2	

514. C₅H₁₁NO₂

D-Valine

β-Amino-isovalerian-saeure

β-Aminoisovaleric acid

RN: 640-68-6 MP (°C): >295

MW: 117.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.291E-02	1.512E+00	10	D038	1 0 1 0 0	EFG, unit assumed, <i>sic</i>
4.296E-01	5.033E+01	20	D041	1 0 0 0 1	
7.053E-01	8.263E+01	25	C018	0 0 0 0 0	
1.343E-02	1.574E+00	25	D038	1 0 1 0 0	EFG, unit assumed, <i>sic</i>
1.384E-02	1.622E+00	33	D038	1 0 1 0 0	EFG, unit assumed, <i>sic</i>
1.426E-02	1.671E+00	40	D038	1 0 1 0 0	EFG, unit assumed, <i>sic</i>
1.455E-02	1.705E+00	49	D038	1 0 1 0 0	EFG, unit assumed, <i>sic</i>
1.500E-02	1.757E+00	57	D038	1 0 1 0 0	EFG, unit assumed, <i>sic</i>
1.592E-02	1.865E+00	65	D038	1 0 1 0 0	EFG, unit assumed, <i>sic</i>

515. C₅H₁₁NO₂

Betaine

Betain

RN: 107-43-7 MP (°C): 296

MW: 117.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.216E+00	6.110E+02	19.30	F300	1 0 0 0 2	

516. C₅H₁₁NO₂

DL-Norvaline

DL-2-Aminovaleric acid

RN: 760-78-1 MP (°C): 303.0

MW: 117.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.251E-01	9.666E+01	15	D041	1 0 0 0 2	
7.768E-01	9.100E+01	18	F300	1 0 0 0 1	
6.616E-01	7.751E+01	25	K031	2 1 2 1 2	

517. C₅H₁₁NO₂

L-Valine

Valine

L-(+)-valine

L-2-Amino-3-methylbutyric acid

2-Amino-3-methylbutyric acid

RN: 72-18-4**MP (°C):** 315**MW:** 117.15**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.180E-01	8.411E+01	15	D349	2 1 1 2 2	
4.866E-01	5.701E+01	20	B032	1 2 2 1 2	
7.360E-01	8.622E+01	20	D349	2 1 1 2 2	
4.992E-01	5.848E+01	25	B032	1 2 2 1 2	
6.940E-01	8.130E+01	25	D041	1 0 0 0 2	
7.550E-01	8.845E+01	25	D349	2 1 1 2 2	
4.710E-01	5.518E+01	25	G092	2 1 1 1 1	
4.710E-01	5.518E+01	25	G315	0 0 0 0 0	
5.900E-01	6.912E+01	25	N001	0 0 0 0 0	EFG
4.740E-01	5.553E+01	25	N012	2 0 2 1 2	
5.019E-01	5.880E+01	27	D036	0 0 0 0 0	
5.114E-01	5.991E+01	29.80	B032	1 2 2 1 2	
7.929E-01	9.289E+01	65	D041	1 0 0 0 2	

518. C₅H₁₁NO₂

3-Nitropentane

Pentane, 3-nitro-

RN: 551-88-2**MP (°C):****MW:** 117.15**BP (°C):** 153

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	1.300E+00	25	A049	1 0 0 0 1	

519. C₅H₁₁NO₂S

DL-Methionine

DL-Methionin

DL-2-Amino-4-(methylthio)butyric acid

Acimetion

RN: 59-51-8**MP (°C):** 281**MW:** 149.21**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	1.790E+01	0	F300	1 0 0 0 2	
1.905E-01	2.843E+01	19.99	F419	0 0 0 0 0	pH 5.81
2.191E-01	3.269E+01	25	D041	1 0 0 0 2	
2.191E-01	3.270E+01	25	F300	1 0 0 0 2	
3.039E-01	4.535E+01	39.99	F419	0 0 0 0 0	pH 5.56 <i>(continued)</i>

519. C₅H₁₁NO₂S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.211E-01	4.791E+01	44.99	F419	0 0 0 0 0	pH 5.51
3.833E-01	5.720E+01	50	F300	1 0 0 0 2	
4.241E-01	6.328E+01	54.99	F419	0 0 0 0 0	pH 5.39
5.596E-01	8.350E+01	69.99	F419	0 0 0 0 0	pH 5.24
6.379E-01	9.519E+01	75	D041	1 0 0 0 2	
6.380E-01	9.520E+01	75	F300	1 0 0 0 2	
6.965E-01	1.039E+02	79.99	F419	0 0 0 0 0	pH 5.15
1.003E+00	1.497E+02	100	F300	1 0 0 0 2	
2.212E-01	3.300E+01	ns	K444	0 0 0 0 0	

520. C₅H₁₁NO₂S

Methionine

L-(-)-Methionine

2-Amino-4-(methylthio)butanoic acid

RN: 63-68-3 MP (°C): -279

MW: 149.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.504E-01	5.228E+01	20	B032	1 2 2 1 2	
3.791E-01	5.656E+01	25	B032	1 2 2 1 2	
3.566E-01	5.321E+01	25	G315	0 0 0 0 0	
3.753E-01	5.600E+01	25.1	N024	0 0 0 0 0	
3.746E-01	5.590E+01	25.1	N026	0 0 0 0 0	
3.548E-01	5.294E+01	25.1	N027	1 1 2 2 2	
3.498E-01	5.220E+01	27	D036	0 0 0 0 0	
4.093E-01	6.107E+01	29.80	B032	1 2 2 1 2	

521. C₅H₁₁NO₂S

Penicillamine

3,3-Dimethyl-D-(-)-cysteine

D-3-Mercaptovaline

D-Penicillamine

RN: 52-67-5 MP (°C): 198.0

MW: 149.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.702E-01	1.000E+02	20	C120	0 0 0 0 0	

522. C₅H₁₁NO₂.H₂O

Betaine (monohydrate)

Trimethylammonioacetate (monohydrate)

RN: 590-47-6 MP (°C):

MW: 135.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.520E+00	6.109E+02	19	D041	1 0 0 0 2	

523. C₅H₁₂

Pentane

n-Pentane

RN: 109-66-0 MP (°C): -130

MW: 72.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.106E-04	6.570E-02	0	P003	2 2 2 2 2	
5.666E-04	4.088E-02	4.0	N004	1 1 2 2 2	
1.516E-04	1.094E-02	4.8	L007	2 1 1 2 2	
1.516E-04	1.094E-02	5.1	L007	2 0 1 1 2	
5.944E-04	4.289E-02	10.0	N004	1 1 2 2 2	
1.635E-04	1.180E-02	14.8	L007	2 1 1 2 2	
2.425E-04	1.750E-02	20	M337	2 1 2 2 2	
5.444E-04	3.928E-02	20.0	N004	1 1 2 2 2	
1.563E-04	1.128E-02	24.8	L007	2 1 1 2 2	
5.267E-04	3.800E-02	25	A049	1 0 0 0 1	
5.475E-04	3.950E-02	25	K119	1 0 0 0 2	
5.336E-04	3.850E-02	25	M001	2 1 2 2 2	
5.336E-04	3.850E-02	25	M002	2 1 2 2 2	
5.650E-04	4.077E-02	25	M342	1 0 1 1 2	
6.597E-04	4.760E-02	25	P003	2 2 2 2 2	
5.611E-04	4.048E-02	25.0	N004	1 1 2 2 2	
5.475E-04	3.950E-02	25.0	P051	2 1 1 2 2	
5.475E-04	3.950E-02	25.00	P007	2 1 2 2 2	
5.611E-04	4.048E-02	30.0	N004	1 1 2 2 2	
1.509E-04	1.089E-02	34.8	L007	2 1 1 2 2	
5.516E-04	3.980E-02	40.1	P051	2 1 1 2 2	
5.516E-04	3.980E-02	40.10	P007	2 1 2 2 2	
5.793E-04	4.180E-02	55.7	P051	2 1 1 2 2	
5.793E-04	4.180E-02	55.70	P007	2 1 2 2 2	
9.619E-04	6.940E-02	99.1	P051	2 1 1 2 2	
9.619E-04	6.940E-02	99.10	P007	2 1 2 2 2	
1.525E-03	1.100E-01	121.3	P051	2 1 1 2 2	
1.525E-03	1.100E-01	121.30	P007	2 1 2 2 2	
2.786E-03	2.010E-01	137.3	P051	2 1 1 2 2	
2.786E-03	2.010E-01	137.30	P007	2 1 2 2 2	
4.130E-03	2.980E-01	149.5	P051	2 1 1 2 2	
4.130E-03	2.980E-01	149.50	P007	2 1 2 2 2	
1.010E-04	7.287E-03	ns	D348	0 0 0 0 0	

524. C₅H₁₂

2-Methylbutane

Isopentane

Izopentan

RN: 78-78-4

MP (°C): -160

MW: 72.15

BP (°C): 30

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-03	7.240E-02	0	P003	2 2 2 2 2	
6.653E-04	4.800E-02	25	K119	1 0 0 0 2	
6.625E-04	4.780E-02	25	M001	2 1 2 2 2	
6.625E-04	4.780E-02	25	M002	2 1 2 2 2	
6.874E-04	4.960E-02	25	P003	2 2 2 2 2	
6.653E-04	4.800E-02	25	P007	2 1 2 2 2	
6.653E-04	4.800E-02	25	P051	2 1 1 2 2	

525. C₅H₁₂

Neopentane

2,2-Dimethylpropane

RN: 463-82-1

MP (°C):

MW: 72.15

BP (°C): 9.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-04	1.602E-02	25	D346	0 0 0 0 0	
4.601E-04	3.320E-02	25	M001	2 1 2 2 2	
5.611E-04	4.048E-02	25	S212	2 1 2 2 2	
3.833E-04	2.766E-02	40	S212	2 1 2 2 1	
2.667E-04	1.924E-02	60	S212	2 1 2 2 1	
2.389E-04	1.724E-02	80	S212	2 1 2 2 1	

526. C₅H₁₂ClO₂PS₂

Chlormephos

Dotan

Diethyl S-(chloromethyl) dithiophosphate

RN: 24934-91-6 MP (°C):

MW: 234.70 BP (°C): 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-04	6.000E-02	20	L303	1 0 0 0 1	
2.556E-04	6.000E-02	20	M161	1 0 0 0 1	
2.559E-04	6.005E-02	ns	S460	0 0 0 0 0	

527. C₅H₁₂NO₃PS₂

Dimethoate

O,O-Dimethyl S-(*N*-methylcarbamoylmethyl) dithiophosphate

RN: 60-51-5 MP (°C): 52.25

MW: 229.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.096E-01	2.514E+01	20	B179	0 0 0 0 0	
1.309E-01	3.000E+01	20	G319	0 0 0 0 0	
1.090E-01	2.500E+01	21	M161	1 0 0 0 1	
1.701E-01	3.900E+01	ns	M061	0 0 0 0 1	

528. C₅H₁₂N₂

2-Methylpiperazine

2-Methyl-piperazin

RN: 109-07-9 MP (°C): 66
MW: 100.16 BP (°C): 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.343E+00	4.350E+02	20	F300	1 0 0 0 2	

529. C₅H₁₂N₂OMethyl-*n*-butylnitrosamine

MBN

RN: 7068-83-9 MP (°C):
MW: 116.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-01	2.323E+01	24	M031	1 1 1 1 1	

530. C₅H₁₂O

2-Methyl-1-butanol

DL-2-Methyl-1-butanol

2-Methylbutan-1-ol

RN: 137-32-6 MP (°C): -70
MW: 88.15 BP (°C): 128.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.269E-01	3.763E+01	.5	S307	1 1 0 2 2	
3.720E-01	3.279E+01	9.7	S307	1 1 0 2 2	
3.122E-01	2.752E+01	19.6	S307	1 1 0 2 2	
3.496E-01	3.082E+01	20	G004	2 2 2 2 2	
3.304E-01	2.913E+01	25	C093	2 1 1 1 1	
3.272E-01	2.884E+01	25	G004	2 2 2 2 2	
2.778E-01	2.449E+01	29.6	S307	1 1 0 2 2	
3.122E-01	2.752E+01	30	G004	2 2 2 2 2	

(continued)

530. C₅H₁₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.616E-01	2.306E+01	39.3	S307	1 1 0 2 2	
2.453E-01	2.162E+01	49.6	S307	1 1 0 2 2	
2.301E-01	2.028E+01	59.3	S307	1 1 0 2 2	
2.485E-01	2.191E+01	69.5	S307	1 1 0 2 2	
2.551E-01	2.248E+01	79.7	S307	1 1 0 2 2	
2.724E-01	2.401E+01	90.8	S307	1 1 0 2 2	

531. C₅H₁₂O

tert-Isoamyl alcohol

3-Methyl-1-butanol

Isopentyl alcohol

Isoamyl alcohol

RN: 123-51-3

MP (°C): -117

MW: 88.15

BP (°C): 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.079E-01	3.596E+01	0	S307	1 1 0 2 2	
3.090E-01	2.724E+01	10	A328	0 0 0 0 0	
3.454E-01	3.044E+01	10.1	S307	1 1 0 2 2	
3.347E-01	2.950E+01	15	K002	1 2 1 1 2	
3.130E-01	2.759E+01	18	F001	1 0 1 2 2	
2.918E-01	2.572E+01	19.8	S307	1 1 0 2 2	
3.120E-01	2.750E+01	20	F300	1 0 0 0 2	
3.144E-01	2.771E+01	20	G004	2 2 2 2 2	
3.111E-01	2.743E+01	20	K002	1 2 1 1 2	
9.586E-01	8.450E+01	20	K085	1 0 0 0 2	
2.659E-01	2.344E+01	25	A328	0 0 0 0 0	
3.411E-01	3.007E+01	25	C068	2 2 2 1 2	
2.982E-01	2.629E+01	25	C093	2 1 1 1 1	
3.251E-01	2.865E+01	25	F317	2 1 1 1 2	
2.950E-01	2.601E+01	25	G004	2 2 2 2 2	
2.950E-01	2.601E+01	25	K002	1 2 1 1 2	
2.799E-01	2.468E+01	30	G004	2 2 2 2 2	
2.832E-01	2.496E+01	30	K002	1 2 1 1 2	
2.842E-01	2.506E+01	30.1	H043	2 2 2 2 2	average of 3
2.540E-01	2.239E+01	30.2	S307	1 1 0 2 2	
2.442E-01	2.153E+01	40	A328	0 0 0 0 0	
2.420E-01	2.133E+01	40.0	S307	1 1 0 2 2	
2.257E-01	1.990E+01	49.9	S307	1 1 0 2 2	
2.431E-01	2.143E+01	59.8	S307	1 1 0 2 2	
2.344E-01	2.066E+01	70.0	S307	1 1 0 2 2	
2.442E-01	2.153E+01	80.0	S307	1 1 0 2 2	
2.518E-01	2.220E+01	90.0	S307	1 1 0 2 2	
2.836E-01	2.500E+01	ns	L003	0 0 2 1 2	
2.767E-01	2.439E+01	rt	H111	0 0 0 0 1	

532. C₅H₁₂O

Neopentyl alcohol

t-Butyl carbinol

RN: 75-84-3

MP (°C): 53

MW: 88.15

BP (°C): 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.048E-01	3.568E+01	12.0	S307	1 1 0 2 2	
3.826E-01	3.372E+01	18.8	S307	1 1 0 2 2	
4.090E-01	3.605E+01	20	G004	2 2 2 2 2	
3.836E-01	3.382E+01	25	G004	2 2 2 2 2	
3.603E-01	3.176E+01	30	G004	2 2 2 2 2	
3.229E-01	2.847E+01	30.0	S307	1 1 0 2 2	
2.982E-01	2.629E+01	40.0	S307	1 1 0 2 2	
2.616E-01	2.306E+01	50.0	S307	1 1 0 2 2	
2.778E-01	2.449E+01	60.0	S307	1 1 0 2 2	
2.399E-01	2.114E+01	70.2	S307	1 1 0 2 2	
2.864E-01	2.525E+01	80.0	S307	1 1 0 2 2	
2.637E-01	2.325E+01	90.0	S307	1 1 0 2 2	

533. C₅H₁₂OMethyl *tert*-butyl ether*tert*-Butyl methyl ether

RN: 1634-04-4

MP (°C): -109

MW: 88.15

BP (°C): 54.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.564E-01	5.786E+01	2.34	S461	0 0 0 0 0	
6.236E-01	5.497E+01	9.99	S461	0 0 0 0 0	
5.196E-01	4.580E+01	20	E019	1 0 1 1 1	
4.738E-01	4.177E+01	24.99	S461	0 0 0 0 0	
5.815E-01	5.126E+01	25	K072	1 0 1 1 1	
5.815E-01	5.126E+01	25	M087	1 1 2 1 2	

534. C₅H₁₂O

3-Pentanol

Pentan-3-ol

Diethyl carbinol

RN: 584-02-1

MP (°C): <25

MW: 88.15

BP (°C): 115.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.704E-01	7.672E+01	0	S307	1 1 0 2 2	
7.382E-01	6.507E+01	10.2	S307	1 1 0 2 2	
6.026E-01	5.312E+01	20	G004	2 2 2 2 2	

(continued)

534. C₅H₁₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.280E-01	5.536E+01	20.0	S307	1 1 0 2 2	
5.505E-01	4.853E+01	25	C093	2 1 1 1 1	
5.556E-01	4.898E+01	25	G004	2 2 2 2 2	
5.144E-01	4.535E+01	30	G004	2 2 2 2 2	
5.730E-01	5.051E+01	30.0	S307	1 1 0 2 2	
4.510E-01	3.975E+01	40.0	S307	1 1 0 2 2	
4.604E-01	4.058E+01	50.0	S307	1 1 0 2 2	
3.889E-01	3.428E+01	60.0	S307	1 1 0 2 2	
3.783E-01	3.335E+01	70.0	S307	1 1 0 2 2	
3.635E-01	3.204E+01	80.0	S307	1 1 0 2 2	
3.773E-01	3.326E+01	90.0	S307	1 1 0 2 2	
1.392E+00	1.227E+02	ns	L003	0 0 2 1 1	
5.196E-01	4.580E+01	rt	H111	0 0 0 0 1	

535. C₅H₁₂O

3-Methyl-2-butanol

Methylisopropylcarbinol

RN: 598-75-4 **MP (°C):** <25
MW: 88.15 **BP (°C):** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.771E-01	7.732E+01	0	S307	1 1 0 2 2	
7.609E-01	6.708E+01	10.1	S307	1 1 0 2 2	
6.492E-01	5.723E+01	20	G004	2 2 2 2 2	
6.381E-01	5.625E+01	20.0	S307	1 1 0 2 2	
5.505E-01	4.853E+01	30	G004	2 2 2 2 2	
5.536E-01	4.880E+01	30.0	S307	1 1 0 2 2	
4.833E-01	4.260E+01	40.0	S307	1 1 0 2 2	
4.416E-01	3.892E+01	50.0	S307	1 1 0 2 2	
3.720E-01	3.279E+01	60.0	S307	1 1 0 2 2	
4.005E-01	3.531E+01	70.0	S307	1 1 0 2 2	
3.942E-01	3.475E+01	79.5	S307	1 1 0 2 2	
3.942E-01	3.475E+01	90.0	S307	1 1 0 2 2	

536. C₅H₁₂O

Ethylisopropyl ether

Propane, 2-ethoxy-

RN: 625-54-7 **MP (°C):**
MW: 88.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-01	2.409E+01	ns	J300	0 0 0 0 0	

537. C₅H₁₂O

1-Pentanol

Amyl alcohol

Pentanol

Pentyl alcohol

n-Amyl alcohol**RN:** 71-41-0**MP (°C):** -79**MW:** 88.15**BP (°C):** 138

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.321E-01	3.809E+01	-5	F051	2 1 0 1 2	
3.358E-01	2.960E+01	0	E029	1 2 0 1 2	
3.635E-01	3.204E+01	0	S307	1 1 0 2 2	
3.709E-01	3.269E+01	7	F051	2 1 0 1 2	
2.982E-01	2.629E+01	10	E029	1 2 0 1 2	
2.864E-01	2.525E+01	10.2	S307	1 1 0 2 2	
3.068E-01	2.705E+01	14	F051	2 1 0 1 2	
3.004E-01	2.648E+01	15	F051	2 1 0 1 2	
5.395E+00	4.756E+02	15.5	F051	2 1 0 1 2	
2.875E-01	2.534E+01	16.5	F051	2 1 0 1 2	
2.821E-01	2.487E+01	18	F051	2 1 0 1 2	
2.453E-01	2.162E+01	20	A015	1 2 1 1 2	
1.020E-02	8.992E-01	20	D052	1 1 0 0 0	<i>sic</i>
2.605E-01	2.296E+01	20	E029	1 2 0 1 2	
2.616E-01	2.306E+01	20	G004	2 2 2 2 2	
1.676E-01	1.478E+01	20	L049	1 1 2 1 1	
3.070E-01	2.706E+01	20	M312	1 0 0 0 1	
2.496E-01	2.200E+01	20.2	S307	1 1 0 2 2	
3.607E-01	3.180E+01	22	H072	1 0 1 1 2	
2.691E-01	2.372E+01	23	F051	2 1 0 1 2	
3.730E-01	3.288E+01	25	B019	1 0 1 2 0	
2.451E-01	2.160E+01	25	B038	1 0 1 1 2	
1.896E-01	1.672E+01	25	B060	2 0 1 1 1	
2.442E-01	2.153E+01	25	C093	2 1 1 1 1	
1.000E+00	8.815E+01	25	F044	1 0 0 0 0	EFG
2.137E-01	1.884E+01	25	F317	2 1 1 1 2	
2.431E-01	2.143E+01	25	G004	2 2 2 2 2	
2.300E-01	2.027E+01	25	G075	1 0 1 0 1	
2.810E-01	2.477E+01	25	H028	2 0 2 0 2	
2.817E-01	2.483E+01	25	H104	1 0 0 0 1	
2.500E-01	2.204E+01	25	K025	2 2 1 1 1	
2.561E-01	2.258E+01	29	F051	2 1 0 1 2	
2.333E-01	2.057E+01	30	E029	1 2 0 1 2	
2.257E-01	1.990E+01	30	G004	2 2 2 2 2	
2.246E-01	1.980E+01	30.6	S307	1 1 0 2 2	
5.368E+00	4.732E+02	34.0	F051	2 1 0 1 2	
2.475E-01	2.181E+01	36	F051	2 1 0 1 2	
2.130E-01	1.878E+01	37	E028	1 0 1 1 2	
2.115E-01	1.865E+01	40	E029	1 2 0 1 2	
2.082E-01	1.836E+01	40.2	S307	1 1 0 2 2	
2.006E-01	1.768E+01	50	E029	1 2 0 1 2	

(continued)

537. C₅H₁₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.039E-01	1.797E+01	50.0	S307	1 1 0 2 2	
2.475E-01	2.181E+01	58	F051	2 1 0 1 2	
2.006E-01	1.768E+01	60	E029	1 2 0 1 2	
2.039E-01	1.797E+01	60.3	S307	1 1 0 2 2	
5.290E+00	4.664E+02	69.5	F051	2 1 0 1 2	
2.061E-01	1.816E+01	70	E029	1 2 0 1 2	
2.170E-01	1.913E+01	70.0	S307	1 1 0 2 2	
2.561E-01	2.258E+01	72.0	F051	2 1 0 1 2	
2.115E-01	1.865E+01	80	E029	1 2 0 1 2	
2.213E-01	1.951E+01	80.0	S307	1 1 0 2 2	
2.691E-01	2.372E+01	81	F051	2 1 0 1 2	
2.821E-01	2.487E+01	87	F051	2 1 0 1 2	
2.224E-01	1.961E+01	90	E029	1 2 0 1 2	
2.453E-01	2.162E+01	90.7	S307	1 1 0 2 2	
2.875E-01	2.534E+01	91	F051	2 1 0 1 2	
3.004E-01	2.648E+01	95	F051	2 1 0 1 2	
5.180E+00	4.566E+02	97.3	F051	2 1 0 1 2	
3.068E-01	2.705E+01	98	F051	2 1 0 1 2	
2.496E-01	2.200E+01	100	E029	1 2 0 1 2	
2.875E-01	2.534E+01	110	E029	1 2 0 1 2	
3.709E-01	3.269E+01	112	F051	2 1 0 1 2	
3.304E-01	2.913E+01	120	E029	1 2 0 1 2	
5.048E+00	4.450E+02	122.3	F051	2 1 0 1 2	
4.321E-01	3.809E+01	126	F051	2 1 0 1 2	
3.889E-01	3.428E+01	130	E029	1 2 0 1 2	
4.677E-01	4.123E+01	140	E029	1 2 0 1 2	
5.351E-01	4.717E+01	140	F051	2 1 0 1 2	
4.896E+00	4.316E+02	141.6	F051	2 1 0 1 2	
5.853E-01	5.159E+01	145	F051	2 1 0 1 2	
6.290E-01	5.545E+01	148.5	F051	2 1 0 1 2	
5.761E-01	5.078E+01	150	E029	1 2 0 1 2	
4.707E+00	4.149E+02	157.3	F051	2 1 0 1 2	
7.322E-01	6.455E+01	160	E029	1 2 0 1 2	
9.060E-01	7.987E+01	167.0	F051	2 1 0 1 2	
9.889E-01	8.717E+01	170	E029	1 2 0 1 2	
1.001E+00	8.826E+01	171.2	F051	2 1 0 1 2	
4.374E+00	3.856E+02	174.0	F051	2 1 0 1 2	
1.690E+00	1.489E+02	180	E029	1 2 0 1 2	
4.089E+00	3.605E+02	181.3	F051	2 1 0 1 2	
1.435E+00	1.265E+02	182.5	F051	2 1 0 1 2	
3.774E+00	3.327E+02	185.2	F051	2 1 0 1 2	
1.833E+00	1.616E+02	186.0	F051	2 1 0 1 2	
2.270E+00	2.001E+02	186.5	F051	2 1 0 1 2	
3.472E+00	3.061E+02	186.5	F051	2 1 0 1 2	
3.237E+00	2.854E+02	187.4	F051	2 1 0 1 2	
3.040E+00	2.680E+02	187.5	F051	2 1 0 1 2	
2.810E-01	2.477E+01	ns	A406	0 0 0 0 1	
2.538E-01	2.237E+01	ns	L003	0 0 2 1 2	
2.224E-01	1.961E+01	rt	H111	0 0 0 0 1	

538. C₅H₁₂O

2-Pentanol

iso-Amyl alcohol*sec*-Amyl alcohol

Methyl propyl carbinol

RN: 6032-29-7

MP (°C): -50

MW: 88.15

BP (°C): 119.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.708E-01	6.795E+01	0	S307	1 1 0 2 2	
6.189E-01	5.455E+01	10.1	S307	1 1 0 2 2	
5.030E-01	4.434E+01	19.5	S307	1 1 0 2 2	
4.573E-01	4.031E+01	20	C042	0 0 0 0 0	
1.473E-02	1.298E+00	20	D052	1 1 0 0 0	<i>sic</i>
4.538E-01	4.000E+01	20	F300	1 0 0 0 1	
5.258E-01	4.635E+01	20	G004	2 2 2 2 2	
3.836E-01	3.382E+01	25	B019	1 0 1 2 0	
4.843E-01	4.270E+01	25	G004	2 2 2 2 2	
4.499E-01	3.966E+01	30	G004	2 2 2 2 2	
4.300E-01	3.791E+01	30.6	S307	1 1 0 2 2	
3.900E-01	3.438E+01	40.0	S307	1 1 0 2 2	
3.645E-01	3.213E+01	50.0	S307	1 1 0 2 2	
3.432E-01	3.026E+01	60.0	S307	1 1 0 2 2	
3.379E-01	2.979E+01	70.1	S307	1 1 0 2 2	
3.443E-01	3.035E+01	79.9	S307	1 1 0 2 2	
3.368E-01	2.969E+01	90.3	S307	1 1 0 2 2	
5.149E-01	4.539E+01	ns	L003	0 0 2 1 2	

539. C₅H₁₂O*tert*-Pentyl alcohol

Dimethylethylcarbinol

tert-Amylalkohol

RN: 75-85-4

MP (°C):

MW: 88.15

BP (°C): 102.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.548E+00	1.364E+02	.5	S307	1 1 0 2 2	
1.462E+00	1.289E+02	9.8	S307	1 1 0 2 2	
1.259E+00	1.110E+02	20	F300	1 0 0 0 2	
1.229E+00	1.083E+02	20	G004	2 2 2 2 2	
1.170E+00	1.031E+02	20.8	S307	1 1 0 2 2	
1.124E+00	9.910E+01	25	G004	2 2 2 2 2	
5.965E-01	5.258E+01	25	G004	2 2 2 2 2	
1.026E+00	9.041E+01	29.5	S307	1 1 0 2 2	
1.041E+00	9.173E+01	30	G004	2 2 2 2 2	
8.549E-01	7.536E+01	39.5	S307	1 1 0 2 2	
7.649E-01	6.743E+01	49.0	S307	1 1 0 2 2	
6.673E-01	5.882E+01	60.0	S307	1 1 0 2 2	
6.391E-01	5.634E+01	70.2	S307	1 1 0 2 2	
6.117E-01	5.393E+01	80.1	S307	1 1 0 2 2	
5.883E-01	5.186E+01	90.2	S307	1 1 0 2 2	
1.124E+00	9.910E+01	rt	H111	0 0 0 0 2	

540. C₅H₁₂O₂

Formaldehyde diethyl acetal

Diethoxymethane

Diethylacetalformaldehyde

Formaldehyd-diaethyl-acetal

RN: 462-95-3 **MP (°C):**
MW: 104.15 **BP (°C):** 87.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.721E-01	7.000E+01	18	F300	1 0 0 0 1	

541. C₅H₁₂O₄

Pentaerythritol

2,2-bis(Hydroxymethyl)-1,3-propanediol

PE 200

Tetramethylolmethane

RN: 115-77-5 **MP (°C):** 260
MW: 136.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-01	3.846E+01	0	M043	1 0 0 0 0	
3.498E-01	4.762E+01	10	M043	1 0 0 0 0	
3.863E-01	5.260E+01	15	F300	1 0 0 0 2	
4.157E-01	5.660E+01	20	M043	1 0 0 0 0	
5.441E-01	7.407E+01	30	M043	1 0 0 0 0	
8.450E-01	1.150E+02	40	M043	1 0 0 0 1	
1.324E+00	1.803E+02	60	M043	1 0 0 0 1	
2.099E+00	2.857E+02	80	M043	1 0 0 0 1	
3.672E+00	5.000E+02	100	M043	1 0 0 0 2	
3.890E-01	5.297E+01	ns	R424	0 0 0 0 0	

542. C₅H₁₂O₅

Adonitol

Adonit

Adonite

RN: 488-81-3 **MP (°C):** 104
MW: 152.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.954E+00	6.016E+02	25	C346	0 0 0 0 0	

543. C₅H₁₂O₅

Xylitol

RN: 87-99-0

MP (°C): 96 K

MW: 152.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.798E+00	5.778E+02	20.12	W414	0 0 0 0 0	
3.963E+00	6.030E+02	25.1	W414	0 0 0 0 0	
4.153E+00	6.319E+02	30.01	W414	0 0 0 0 0	
4.355E+00	6.627E+02	35.05	W414	0 0 0 0 0	
4.550E+00	6.922E+02	40.13	W414	0 0 0 0 0	
4.721E+00	7.183E+02	45.10	W414	0 0 0 0 0	
4.873E+00	7.414E+02	50.09	W414	0 0 0 0 0	
5.001E+00	7.610E+02	55.05	W414	0 0 0 0 0	

544. C₅H₁₂O₅

DL-Arabinitol

(±)-Arabitol

RN: 2152-56-9

MP (°C): 103

MW: 152.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.459E+00	6.785E+02	25	C346	0 0 0 0 0	

545. C₅H₁₃N

N-Methyldiethylamine

N,N-Diethylmethylamine

RN: 616-39-7

MP (°C):

MW: 87.17

BP (°C): 63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.562E+00	3.105E+02	49.40	C086	2 2 2 2 2	average of 5
4.453E+00	3.881E+02	49.50	C086	2 2 2 2 2	
2.236E+00	1.949E+02	49.80	C086	2 2 2 2 2	
5.715E+00	4.982E+02	50.50	C086	2 2 2 2 2	
1.581E+00	1.378E+02	51.20	C086	2 2 2 2 2	
1.413E+00	1.231E+02	52.00	C086	2 2 2 2 2	
6.981E+00	6.085E+02	53.10	C086	2 2 2 2 2	
7.246E+00	6.316E+02	54.00	C086	2 2 2 2 2	

546. C₅H₁₃O₃PS₂

Demephion

O,O-Dimethyl 2-methylmercaptoethyl thiophosphate

Thiolo-tinox

RN: 8065-62-1 MP (°C):

MW: 216.26 BP (°C): 109

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.312E-03	5.000E-01	20	M061	1 0 0 0 2	form II
9.248E-03	2.000E+00	ns	M061	0 0 0 0 2	form I
1.387E-02	3.000E+00	rt	M161	0 0 0 0 0	form II
1.387E-03	3.000E-01	rt	M161	0 0 0 0 2	form I

547. C₅Cl₆

Hexachlorocyclopentadiene

1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene

Hexachloro-1,3-cyclopentadiene

1,2,3,4,5,5-Hexachlorocyclopentadiene

RN: 77-47-4 MP (°C): -9.9

MW: 272.77 BP (°C): 239

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-06	8.050E-04	22.5	G301	0 0 0 0 0	

548. C₆HCl₃N₂S

4,5,7-Trichloro-2,1,3-benzothiadiazole

PH 40-21

TH 052 H

RN: 1982-55-4 MP (°C): 131.5

MW: 239.51 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.263E-06	1.500E-03	10	B200	1 0 0 0 1	
1.044E-05	2.500E-03	20	B200	1 0 0 0 1	
1.044E-05	2.500E-03	20	M061	1 0 0 0 1	
1.795E-05	4.300E-03	30	B200	1 0 0 0 1	

549. C₆HCl₄NO₂

2,3,4,5-Tetrachloronitrobenzene

1,2,3,4-Tetrachloro-5-nitrobenzene

2,3,4,5-Tetrachloro-1-nitrobenzene

1-Nitro-2,3,4,5-tetrachlorobenzene

RN: 879-39-0 MP (°C): 66.0

MW: 260.89 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	7.305E-03	20	E308	1 2 2 1 1	

550. C₆HCl₄NO₂

2,3,4,6-Tetrachloronitrobenzene

Benzene, 1,2,3,5-tetrachloro-4-nitro-

RN: 3714-62-3 MP (°C):

MW: 260.89 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-05	7.566E-03	20	E308	1 2 2 1 1	

551. C₆HCl₄NO₂

2,3,5,6-Tetrachloronitrobenzene

Tecnazene

RN: 117-18-0 MP (°C): 99.5
MW: 260.89 BP (°C): 304.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-06	2.087E-03	20	E308	1 2 2 1 0	

552. C₆HCl₅

Pentachlorobenzene

Penta-chlorobenzene

RN: 608-93-5 MP (°C): 82
MW: 250.34 BP (°C): 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-06	2.503E-04	20	K337	1 0 0 0 2	
9.550E-07	2.391E-04	22	K305	1 0 1 1 0	
1.538E-06	3.850E-04	23	C305	1 1 2 2 2	
5.320E-06	1.332E-03	25	B173	2 0 2 2 2	
2.600E-06	6.509E-04	25	B317	0 0 0 0 0	
3.320E-06	8.311E-04	25	M342	1 0 1 1 2	
3.320E-06	8.311E-04	ns	M308	0 0 1 1 2	

553. C₆HCl₅O

Pentachlorophenol

PCP

2,3,4,5,6-Pentachloro-phenol-

Phenol, 2,3,4,5,6-pentachloro-

Dowicide 7

Fungifen

RN: 87-86-5 MP (°C): 174
MW: 266.34 BP (°C): 310

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.877E-05	5.000E-03	0	C310	0 0 0 0 0	
1.877E-05	5.000E-03	0	G310	1 0 0 0 0	
1.877E-05	5.000E-03	0	M061	1 0 0 0 0	

(continued)

553. C₆HCl₅O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.256E-05	1.400E-02	20	B185	0 0 0 0 0	
5.256E-05	1.400E-02	22.5	G301	0 0 0 0 0	
6.195E-05	1.650E-02	25	B183	0 0 0 0 1	
8.260E-05	2.200E-02	25	B185	0 0 0 0 0	
3.600E-05	9.588E-03	25	B316	0 0 0 0 0	
6.908E-05	1.840E-02	25	M373	1 0 2 1 2	
5.256E-05	1.400E-02	25	O320	0 0 0 0 0	
8.035E-05	2.140E-02	25.1	A400	2 1 2 2 2	
5.256E-05	1.400E-02	26.70	L095	2 2 1 1 2	
6.758E-05	1.800E-02	27	C310	0 0 0 0 0	
6.758E-05	1.800E-02	27	G310	1 0 0 0 1	
6.758E-05	1.800E-02	27	M061	1 0 0 0 1	
3.484E-03	9.280E-01	30	A400	2 1 2 2 2	
7.509E-05	2.000E-02	30	M161	1 0 0 0 1	
1.126E-04	3.000E-02	50	B200	1 0 0 0 0	
1.314E-04	3.500E-02	50	C310	0 0 0 0 0	
1.314E-04	3.500E-02	50	G310	1 0 0 0 1	
1.314E-04	3.500E-02	50	M061	1 0 0 0 1	
2.178E-04	5.800E-02	62	C310	0 0 0 0 0	
2.178E-04	5.800E-02	62	G310	1 0 0 0 1	
3.191E-04	8.499E-02	70	C310	0 0 0 0 0	
3.191E-04	8.499E-02	70	G310	1 0 0 0 1	
7.509E-05	2.000E-02	ns	L311	0 0 0 0 1	
7.134E-05	1.900E-02	ns	M110	0 0 0 0 0	EFG
6.007E-06	1.600E-03	ns	N013	0 0 0 0 1	

554. C₆HF₅O

Pentafluorophenol

PFP

RN: 771-61-9 **MP (°C):** 34–36
MW: 184.07 **BP (°C):** 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-01	5.522E+01	25	P031	0 0 0 0 0	

555. C₆H₂Br₂ClNO₂

2,6-Dibromoquinone-3-chlorimide

2,6-Dibromoquinonechloroimide

RN: **MP (°C):**
MW: 315.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	6.307E-02	20	G043	1 0 1 1 0	

556. C₆H₂Br₄

1,2,4,5-Tetrabromobenzene

RN: 636-28-2

MP (°C):

MW: 393.72

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.724E-08	1.860E-05	10	K440	0 0 0 0 0	
1.105E-07	4.350E-05	25	K440	0 0 0 0 0	
1.976E-07	7.780E-05	35	K440	0 0 0 0 0	

557. C₆H₂ClN₃O₆

2,4,6-Trinitro-1-chlorobenzene

Picryl chloride

2-Chlor-1,3,5-trinitrobenzol

Chlorure de picryle

RN: 88-88-0

MP (°C):

MW: 247.55

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.190E-04	1.780E-01	15	D066	1 2 0 0 2	
7.189E-04	1.780E-01	15	D071	1 2 0 0 2	
7.271E-04	1.800E-01	15	F300	1 0 0 0 1	
2.141E-03	5.300E-01	16	D066	1 2 0 0 2	
2.140E-03	5.297E-01	50	D071	1 2 0 0 1	
1.398E-02	3.460E+00	100	D066	1 2 0 0 2	
1.393E-02	3.448E+00	100	D071	1 2 0 0 2	
1.454E-02	3.600E+00	100	F300	1 0 0 0 1	

558. C₆H₂Cl₂O₄

Chloranilic acid

Chloranilsaeure

RN: 87-88-7

MP (°C): 283

MW: 208.99

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.091E-03	1.900E+00	14	F300	1 0 0 0 1	
6.699E-02	1.400E+01	99	F300	1 0 0 0 1	

559. C₆H₂Cl₃NO₂

2,4,5-Trichloronitrobenzene

1,2,4-Trichloro-5-nitrobenzene

2,4,5-Trichloro-1-nitrobenzene

1,4,5-Trichloro-2-nitrobenzene

3,4,6-Trichloronitrobenzene

RN: 89-69-0

MP (°C): 57

MW: 226.45

BP (°C): 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	2.944E-02	20	E308	1 2 2 1 2	

560. C₆H₂Cl₃NO₂

2,3,4-Trichloronitrobenzene

1,2,3-Trichloro-4-nitrobenzene

2,3,4-Trichloro-1-nitrobenzene

RN: 17700-09-3 **MP (°C):** 55.5**MW:** 226.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-04	2.604E-02	20	E308	1 2 2 1 2	

561. C₆H₂Cl₄

1,2,4,5-Tetrachlorobenzene

s-Tetrachlorobenzene**RN:** 95-94-3 **MP (°C):** 139**MW:** 215.89 **BP (°C):** 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.445E-06	3.121E-04	20	K337	1 0 0 0 2	
1.349E-06	2.912E-04	22	K305	1 0 1 1 1	
2.154E-06	4.650E-04	25	B304	2 0 2 2 2	
5.900E-06	1.274E-03	25	B317	0 0 0 0 0	
1.090E-05	2.353E-03	25	M342	1 0 1 1 2	
1.600E-06	3.454E-04	25.2	T428	0 0 0 0 0	
1.806E-06	3.900E-04	ns	B393	0 0 0 0 0	
1.090E-05	2.353E-03	ns	M308	0 0 1 1 2	

562. C₆H₂Cl₄

Trichlorobenzyl chloride

TCBC

RN: 1344-32-7 **MP (°C):****MW:** 215.89 **BP (°C):** 93

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.264E-06	2.000E-03	25	B200	1 0 0 0 0	

563. C₆H₂Cl₄

1,2,3,4-Tetrachlorobenzene

Benzene, 1,2,3,4-tetrachloro-

RN: 634-66-2 **MP (°C):** 48**MW:** 215.89 **BP (°C):** 254

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-05	3.422E-03	20	K337	1 0 0 0 2	
3.326E-05	7.180E-03	23	C305	1 1 2 2 2	
2.742E-05	5.920E-03	25	B304	2 0 2 2 2	
3.600E-05	7.772E-03	25	B317	0 0 0 0 0	
5.650E-05	1.220E-02	25	M342	1 0 1 1 2	
5.650E-05	1.220E-02	ns	M308	0 0 1 1 2	

564. C₆H₂Cl₄

1,2,3,5-Tetrachlorobenzene

1,2,4,6-Tetrachlorobenzene

RN: 634-90-2 **MP (°C):** 50
MW: 215.89 **BP (°C):** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	2.159E-03	20	K337	1 0 0 0 2	
1.148E-05	2.479E-03	22	K305	1 0 1 1 2	
1.496E-05	3.230E-03	23	C305	1 1 2 2 2	
1.860E-05	4.016E-03	25	B173	2 0 2 2 2	
2.362E-05	5.100E-03	25	B304	2 0 2 2 2	
1.660E-05	3.584E-03	25	B317	0 0 0 0 0	
1.340E-05	2.893E-03	25	M342	1 0 1 1 2	
1.654E-05	3.570E-03	ns	H123	0 0 0 0 0	
1.340E-05	2.893E-03	ns	M308	0 0 1 1 2	

565. C₆H₂Cl₄O

2,3,4,6-Tetrachlorophenol

Phenol, 2,3,4,6-tetrachloro-

1-Hydroxy-2,3,4,6-tetrachlorobenzene

TCP

RN: 58-90-2 **MP (°C):**
MW: 231.89 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.900E-04	1.832E-01	25	B316	0 0 0 0 0	

566. C₆H₂Cl₄O

2,3,4,5-Tetrachlorophenol

Phenol, 2,3,4,5-tetrachloro-

RN: 4901-51-3 **MP (°C):** 116
MW: 231.89 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.158E-04	1.660E-01	25	M373	1 0 2 1 2	

567. C₆H₂Cl₄O

2,3,5,6-Tetrachlorophenol

Phenol, 2,3,5,6-tetrachloro-

RN: 935-95-5 **MP (°C):** 115
MW: 231.89 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.312E-04	1.000E-01	25	M373	1 0 2 1 2	

568. C₆H₂Cl₄O₂

Tetrachlorohydroquinone

2,3,5,6-Tetrachlorohydroquinone

RN: 87-87-6 MP (°C):

MW: 247.89 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.673E-05	2.150E-02	ns	L311	0 0 0 0 1	

569. C₆H₂F₄

1,2,4,5-Tetrafluorobenzene

2,3,5,6-Tetrafluorobenzene

p-Tetrafluorobenzene

RN: 327-54-8 MP (°C): 4.5

MW: 150.08 BP (°C): 89.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.215E-03	6.326E-01	25	B349	2 0 2 0 2	

570. C₆H₂F₄

1,2,3,5-Tetrafluorobenzene

1,2,4,6-Tetrafluorobenzene

m-Tetrafluorobenzene

1,3,4,5-Tetrafluorobenzene

RN: 2367-82-0 MP (°C): -48

MW: 150.08 BP (°C): 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.952E-03	7.431E-01	25	B349	2 0 2 0 2	

571. C₆H₂F₄O

2,3,5,6-Tetrafluorophenol

1,2,4,5-Tetrafluoro-3-hydroxybenzene

RN: 769-39-1 MP (°C): 38

MW: 166.08 BP (°C): 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-01	6.145E+01	25	P031	0 0 0 0 0	

572. C₆H₃Br₂NO₂

2,6-Dibromoquinone oxime

RN: **MP (°C):**
MW: 280.91 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-04	2.388E-01	20	G066	1 0 0 0 1	

573. C₆H₃Br₃

1,2,4-Tribromobenzene

Tribromobenzene, 1,2,4-

RN: 615-54-3 **MP (°C):** 43
MW: 314.82 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.166E-05	3.670E-03	10	K440	0 0 0 0 0	
2.290E-05	7.210E-03	25	K440	0 0 0 0 0	
3.494E-05	1.100E-02	35	K440	0 0 0 0 0	

574. C₆H₃Br₃O

2,4,6-Tribromobiphenyl

1,1'-Biphenyl, 2,4,6-tribromo-

RN: 59080-33-0 **MP (°C):** 66
MW: 330.82 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.111E-02	1.360E+01	26.5	G312	0 0 0 0 0	

575. C₆H₃Br₃O

2,4,6-Tribromophenol

2,4,6-Tribromophenol

Tribromophenol

Bromol

RN: 118-79-6 **MP (°C):** 95
MW: 330.82 **BP (°C):** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.116E-04	7.000E-02	15	F300	1 0 0 0 1	
2.300E-04	7.609E-02	ns	O310	0 0 0 0 1	

576. C₆H₃ClN₂O₄

1-Chloro-2,4-dinitrobenzene

2,4-Dinitro-1-chlorobenzene

4-Chlor-1,3-dinitrobenzol

4-Chloro-1,3-dinitrobenzene

RN: 97-00-7 MP (°C): 53

MW: 202.55 BP (°C): 315

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.950E-05	8.000E-03	15	D071	1 2 0 0 0	
3.950E-05	8.000E-03	15	F300	1 0 0 0 0	
4.560E-05	9.236E-03	25	G090	2 2 1 1 1	
2.023E-03	4.098E-01	50	D071	1 2 0 0 1	
7.837E-03	1.587E+00	100	D071	1 2 0 0 2	
8.393E-03	1.700E+00	100	F300	1 0 0 0 1	
7.244E-04	1.467E-01	ns	R427	0 0 0 0 0	

577. C₆H₃ClN₄

7-Chloropteridine

Pteridine, 7-chloro-

RN: 1125-84-4 MP (°C): 95

MW: 166.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-01	2.174E+01	20	A083	1 2 0 0 0	

578. C₆H₃Cl₂NO₂

3,4-Dichloronitrobenzene

1,2-Dichloro-4-nitrobenzene

RN: 99-54-7 MP (°C): 41.25

MW: 192.00 BP (°C): 255.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.290E-04	1.208E-01	20	E308	1 2 2 1 2	

579. C₆H₃Cl₂NO₂

2,5-Dichloronitrobenzene

1,4-Dichloro-2-nitrobenzene

RN: 89-61-2 MP (°C): 55.5

MW: 192.00 BP (°C): 267.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-04	9.216E-02	20	E308	1 2 2 1 2	

580. C₆H₃Cl₂NO₂

2,3-Dichloronitrobenzene

1,2-Dichloro-3-nitrobenzene

RN: 3209-22-1 **MP (°C):** 61.5
MW: 192.00 **BP (°C):** 257.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.250E-04	6.240E-02	20	E308	1 2 2 1 2	

581. C₆H₃Cl₂NO₂

3,6-Dichloropicolinic acid

3,6-Dichloro-2-pyridinecarboxylic acid

Clopypralid

Lontrel

Stinger

RN: 1702-17-6 **MP (°C):** 151.5
MW: 192.00 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.208E-03	1.000E+00	20	M161	1 0 0 0 0	
5.208E-03	1.000E+00	ns	K138	0 0 0 0 1	

582. C₆H₃Cl₃

1,2,3-Trichlorobenzene

Benzene, 1,2,3-trichloro-
vic-Trichlorobenzene

RN: 87-61-6 **MP (°C):** 51
MW: 181.45 **BP (°C):** 219

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.762E-05	1.408E-02	20	K337	1 0 0 0 2	
6.607E-05	1.199E-02	22	K305	1 0 1 1 2	
8.983E-05	1.630E-02	23	C305	1 1 2 2 2	
9.920E-05	1.800E-02	25	B304	2 0 2 2 2	
1.170E-04	2.123E-02	25	B317	0 0 0 0 0	
9.920E-05	1.800E-02	25	C313	0 0 0 0 0	
6.760E-05	1.227E-02	25	M342	1 0 1 1 2	
9.149E-05	1.660E-02	ns	H123	0 0 0 0 0	
6.760E-05	1.227E-02	ns	M308	0 0 1 1 2	

583. C₆H₃Cl₃

1,3,5-Trichlorobenzene

Benzene, 1,3,5-trichloro-

RN: 108-70-3 **MP (°C):** 64
MW: 181.45 **BP (°C):** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.399E-05	4.353E-03	20	K337	1 0 0 0 2	
3.236E-05	5.872E-03	22	K305	1 0 1 1 2	
5.842E-05	1.060E-02	23	C305	1 1 2 2 2	
3.312E-05	6.010E-03	25	B304	2 0 2 2 2	
2.900E-05	5.262E-03	25	B317	0 0 0 0 0	
2.270E-05	4.119E-03	25	M342	1 0 1 1 2	
2.270E-05	4.119E-03	ns	M308	0 0 1 1 2	

584. C₆H₃Cl₃

1,2,4-Trichlorobenzene

Benzene, 1,2,4-trichloro-

RN: 120-82-1 **MP (°C):** 17
MW: 181.45 **BP (°C):** 213

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-04	3.000E-02	19	M172	1 0 0 0 0	
1.950E-04	3.538E-02	20	K337	1 0 0 0 2	
1.072E-04	1.944E-02	22	K305	1 0 1 1 2	
1.725E-04	3.130E-02	25	B304	2 0 2 2 2	
2.200E-04	3.992E-02	25	B317	0 0 0 0 0	
2.692E-04	4.884E-02	25	C113	1 0 2 2 2	
2.540E-04	4.609E-02	25	M342	1 0 1 1 2	
3.555E-04	6.451E-02	30	M300	1 1 2 2 2	
3.555E-04	6.450E-02	30	M311	1 1 2 2 2	
2.540E-04	4.609E-02	ns	M308	0 0 1 1 2	

585. C₆H₃Cl₃N₂O₂

Picloram

4-Amino-3,5,6-trichloropicolinic acid

RN: 1918-02-1 **MP (°C):** 241
MW: 241.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.967E-03	4.750E-01	10	C031	2 0 2 2 2	pH 2.8
2.260E-03	5.457E-01	20	C031	2 0 2 2 2	pH 2.8
1.781E-03	4.300E-01	25	B185	0 0 0 0 0	
1.781E-03	4.300E-01	25	B200	1 0 0 0 1	
1.781E-03	4.300E-01	25	M161	1 0 0 0 2	
2.830E-03	6.833E-01	30	C031	2 0 2 2 2	pH 2.8
3.290E-03	7.944E-01	40	C031	2 0 2 2 2	pH 2.8
1.781E-03	4.300E-01	ns	K138	0 0 0 0 1	
1.780E-03	4.298E-01	ns	M061	0 0 0 0 1	
3.500E-04	8.451E-02	ns	O025	2 2 2 2 1	intrinsic

586. C₆H₃Cl₃O

2,3,4-Trichlorophenol

2,3,4-Trichlorophenol

RN: 15950-66-0 MP (°C): 80

MW: 197.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.634E-03	9.150E-01	25	M373	1 0 2 1 2	
2.138E-03	4.221E-01	ns	R424	0 0 0 0 0	

587. C₆H₃Cl₃O

2,3,5-Trichlorophenol

2,3,5-Trichlorophenol

RN: 933-78-8 MP (°C): 62

MW: 197.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.905E-03	7.710E-01	25	M373	1 0 2 1 2	

588. C₆H₃Cl₂O

2,3,6-Trichlorophenol

2,3,6-Trichlorophenol

RN: 933-75-5 MP (°C): 58

MW: 197.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.993E-03	5.910E-01	25	M373	1 0 2 1 2	

589. C₆H₃Cl₃O

2,4,6-Trichlorophenol

2,4,6-Trichlorophenol

Dowicide 25

RN: 88-06-2 MP (°C): 69

MW: 197.45 BP (°C): 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.532E-03	5.000E-01	11.20	F300	1 0 0 0 0	
2.076E-03	4.100E-01	19.5	A400	2 1 2 2 2	
2.163E-03	4.270E-01	20.1	A400	2 1 2 2 2	
4.558E-03	9.000E-01	22.5	G301	0 0 0 0 0	
3.505E-03	6.920E-01	24.9	A400	2 1 2 2 2	
2.200E-03	4.344E-01	25	B316	0 0 0 0 0	
3.586E-03	7.080E-01	25	M373	1 0 2 1 2	
4.554E-03	8.992E-01	25	R041	0 0 0 0 0	
4.558E-03	9.000E-01	25.40	F300	1 0 0 0 0	

(continued)

589. C₆H₃Cl₃O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.077E-02	6.075E+00	29.8	A400	2 1 2 2 2	
3.292E-02	6.501E+00	35.1	A400	2 1 2 2 2	
1.266E-02	2.500E+00	96	F300	1 0 0 0 1	
<5.06E-03	<9.99E-01	ns	N034	0 0 0 0 0	
3.981E-03	7.861E-01	ns	R427	0 0 0 0 0	

590. C₆H₃Cl₃O

2,4,5-Trichloro-phenol

Phenol, 2,4,5-trichloro-

Dowicide 2

Preventol I

2,4,5-Trichlorophenol

Collunosol

RN: 95-95-4

MP (°C): 69

MW: 197.45

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-03	9.478E-01	25	B316	0 0 0 0 0	
3.287E-03	6.490E-01	25	M373	1 0 2 1 2	

591. C₆H₃Cl₄N

Nitrapyrin

2-Chloro-6-(trichloromethyl)pyridine

Donco-163

N-Serve(R)

RN: 1929-82-4

MP (°C): 62.5

MW: 230.91

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.738E-04	4.013E-02	20	B179	0 0 0 0 0	
1.732E-04	4.000E-02	20	G079	1 1 0 0 2	
3.118E-04	7.200E-02	ns	V414	0 0 0 0 0	

592. C₆H₃FN₂O₄

1-Fluoro-2,4-dinitrobenzene

FDNB

RN: 70-34-8

MP (°C): 26

MW: 186.10

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.149E-03	4.000E-01	ns	B160	0 0 0 0 2	

593. C₆H₃F₃O

Trifluorophenol

2,3,4-Trifluorophenol

RN: 2822-41-5 **MP (°C):**
MW: 148.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-01	6.220E+01	25	P031	0 0 0 0 0	

594. C₆H₃N₃O₆

sym-Trinitrobenzene

1,3,5-Trinitro-benzol

1,3,5-Trinitrobenzene

RN: 99-35-4 **MP (°C):** 122.5
MW: 213.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-03	2.780E-01	15	D066	1 2 0 0 2	
1.304E-03	2.779E-01	15	D070	1 2 0 0 2	
1.314E-03	2.800E-01	15	F300	1 0 0 0 1	
1.678E-03	3.577E-01	25	H434	0 0 0 0 0	
4.786E-03	1.020E+00	50	D066	1 2 0 0 2	
4.781E-03	1.019E+00	50	D070	1 2 0 0 2	
2.337E-02	4.980E+00	100	D066	1 2 0 0 2	
2.325E-02	4.955E+00	100	D070	1 2 0 0 2	
2.393E-02	5.100E+00	100	F300	1 0 0 0 1	
1.288E-03	2.745E-01	ns	R427	0 0 0 0 0	

595. C₆H₃N₃O₇

Picric acid

2,4,6-Trinitrophenol

Picronitric acid

Pikrinsaeure

RN: 88-89-1 **MP (°C):** 122.5
MW: 229.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.948E-02	6.754E+00	0	D077	1 0 0 1 1	
4.322E-02	9.901E+00	0	M043	1 0 0 0 1	
4.364E-02	9.999E+00	7.10	E032	1 2 1 2 2	
4.232E-02	9.695E+00	9	D080	1 2 0 0 2	unit assumed
3.507E-02	8.035E+00	10	D077	1 0 0 1 1	
4.749E-02	1.088E+01	10	M043	1 0 0 0 1	
4.407E-02	1.010E+01	18.90	E032	1 2 1 2 2	
4.792E-02	1.098E+01	20	D077	1 0 0 1 2	
5.151E-02	1.180E+01	20	H048	1 0 0 0 2	unit assumed
4.300E-02	9.852E+00	20	K310	1 0 0 1 1	

(continued)

595. C₆H₃N₃O₇ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.176E-02	1.186E+01	20	M043	1 0 0 0 1	
4.932E-02	1.130E+01	23.50	F300	0 0 0 0 2	
5.327E-02	1.220E+01	25	D058	1 0 1 1 2	
5.520E-02	1.265E+01	25	F030	1 0 2 1 2	
5.684E-02	1.302E+01	25	H048	1 0 0 0 2	unit assumed
5.780E-02	1.324E+01	25	K040	1 0 2 1 2	
5.474E-02	1.254E+01	25	M094	1 0 0 1 2	
6.026E-02	1.381E+01	30	D077	1 0 0 1 2	
6.450E-02	1.478E+01	30	M043	1 0 0 0 1	
7.465E-02	1.710E+01	33.30	E032	1 2 1 2 2	
7.633E-02	1.749E+01	40	D077	1 0 0 1 2	
8.138E-02	1.865E+01	40	M043	1 0 0 0 1	
9.396E-02	2.153E+01	44.30	E032	1 2 1 2 2	
9.354E-02	2.143E+01	50	D077	1 0 0 1 2	
9.930E-02	2.275E+01	50	D080	1 2 0 0 2	unit assumed
1.193E-01	2.733E+01	60	D077	1 0 0 1 2	
1.312E-01	3.007E+01	60	M043	1 0 0 0 1	
1.398E-01	3.204E+01	62.90	E032	1 2 1 2 2	
1.464E-01	3.354E+01	70	D077	1 0 0 1 2	
1.703E-01	3.902E+01	72.60	E032	1 2 1 2 2	
1.844E-01	4.224E+01	80	D077	1 0 0 1 2	
1.920E-01	4.398E+01	80	M043	1 0 0 0 1	
1.956E-01	4.481E+01	82	D080	1 2 0 0 2	unit assumed
2.007E-01	4.598E+01	83.90	E032	1 2 1 2 2	
2.362E-01	5.411E+01	90	D077	1 0 0 1 2	
2.160E-01	4.949E+01	90	K310	1 0 0 1 2	
2.244E-01	5.141E+01	90.10	E032	1 2 1 2 2	
2.326E-01	5.330E+01	92.40	E032	1 2 1 2 2	
2.517E-01	5.767E+01	94.80	E032	1 2 1 2 2	
2.947E-01	6.751E+01	100	D077	1 0 0 1 2	
3.083E-01	7.063E+01	100	D080	1 2 0 0 2	unit assumed
3.055E-01	7.000E+01	100	F300	1 0 0 0 1	
2.932E-01	6.716E+01	100	M043	1 0 0 0 1	

596. C₆H₃N₃O₈

Styphnic acid

Styphninsaeure

RN: 82-71-3

MP (°C): 176

MW: 245.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.393E-02	5.865E+00	6.10	E032	1 2 1 2 2	
2.167E-02	5.312E+00	16.60	E032	1 2 1 2 2	
2.203E-02	5.400E+00	25	F300	1 0 0 0 1	
2.179E-02	5.341E+00	25	K040	1 0 2 1 2	
2.997E-02	7.346E+00	35.70	E032	1 2 1 2 2	
3.471E-02	8.507E+00	47.10	E032	1 2 1 2 2	

(continued)

596. C₆H₃N₃O₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.119E-02	1.010E+01	56.90	E032	1 2 1 2 2	
4.692E-02	1.150E+01	62	F300	1 0 0 0 2	
4.758E-02	1.166E+01	63.00	E032	1 2 1 2 2	
6.109E-02	1.497E+01	71.20	E032	1 2 1 2 2	
7.135E-02	1.749E+01	76.20	E032	1 2 1 2 2	
8.000E-02	1.961E+01	80.30	E032	1 2 1 2 2	
9.562E-02	2.344E+01	85.00	E032	1 2 1 2 2	
1.096E-01	2.686E+01	89.80	E032	1 2 1 2 2	
1.357E-01	3.326E+01	95.90	E032	1 2 1 2 2	

597. C₆H₄BrF

1-Bromo-2-fluorobenzene

2-Bromofluorobenzene

RN: 1072-85-1 MP (°C):
 MW: 175.01 BP (°C): 151.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.018E-03	3.532E-01	25	B349	2 0 2 0 2	

598. C₆H₄BrF

1-Bromo-3-fluorobenzene

3-Bromofluorobenzene

RN: 1073-06-9 MP (°C):
 MW: 175.01 BP (°C): 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.162E-03	3.784E-01	25	B349	2 0 2 0 2	

599. C₆H₄BrNO₃

2-Bromo-4-nitrophenol

2-Brom-4-nitro-phenol

RN: 5847-59-6 MP (°C): 114
 MW: 218.01 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	2.200E+01	100	F300	1 0 0 0 1	

600. C₆H₄Br₂*m*-Dibromobenzene

1,3-Dibromobenzene

RN: 108-36-1 **MP (°C):** -7
MW: 235.92 **BP (°C):** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-04	6.747E-02	35	H077	2 2 2 2 2	

601. C₆H₄Br₂*p*-Dibromobenzene

1,4-Dibromobenzene

RN : 106-37-6 **MP (°C):** 87.3
MW: 235.92 **BP (°C):** 220.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.201E-05	9.910E-03	10	K440	0 0 0 0 0	
8.478E-05	2.000E-02	25	A003	1 0 1 2 1	
5.900E-03	1.392E+00	25	C316	0 0 0 0 0	0.1M NaCl
7.206E-05	1.700E-02	25	K440	0 0 0 0 0	
1.120E-04	2.642E-02	35	H077	2 2 2 2 2	
1.043E-04	2.460E-02	35	K440	0 0 0 0 0	

602. C₆H₄ClF

1-Chloro-2-fluorobenzene

2-Chlorofluorobenzene

RN: 348-51-6 **MP (°C):** -43
MW: 130.55 **BP (°C):** 137.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.845E-03	5.019E-01	25	B349	2 0 2 0 2	

603. C₆H₄ClF

1-Chloro-3-fluorobenzene

3-Chlorofluorobenzene

RN: 625-98-9 **MP (°C):**
MW: 130.55 **BP (°C):** 127.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.517E-03	5.897E-01	25	B349	2 0 2 0 2	

604. C₆H₄ClO₂S

Pipsyl chloride

p-Iodobenzenesulfonyl chloride

RN: 98-61-3 MP (°C): 81
 MW: 302.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.388E-05	1.630E-02	25	B048	1 0 2 2 2	
8.793E-05	2.660E-02	35	B048	1 0 2 2 2	
1.646E-04	4.980E-02	50	B048	1 0 2 2 2	

605. C₆H₄CINO₂

6-Chloropicolinic acid

Pyridinecarboxylic acid, 6-chloro-

RN: 4684-94-0 MP (°C):
 MW: 157.56 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.158E-02	3.400E+00	ns	K138	0 0 0 0 1	
2.138E-02	3.369E+00	ns	R427	0 0 0 0 0	

606. C₆H₄CINO₂*p*-Chloronitrobenzene

4-Nitrochlorobenzene

4-CNB

4-Chloronitrobenzene

RN: 100-00-5 MP (°C): 82
 MW: 157.56 BP (°C): 242

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.711E-04	1.530E-01	9.99	B403	1 2 2 2 2	
1.777E-04	2.800E-02	17	D071	1 2 0 0 1	
1.777E-04	2.800E-02	17	F300	1 0 0 0 1	
1.327E-03	2.090E-01	19.99	B403	1 2 2 2 2	
2.877E-03	4.533E-01	20	E308	1 2 2 1 2	
1.429E-03	2.251E-01	20	H118	1 1 1 1 2	
1.429E-03	2.251E-01	20	H301	0 0 0 0 0	
<1.27E-03	<2.00E-01	25	B019	1 0 1 2 0	
1.600E-03	2.521E-01	25	G090	2 2 1 1 1	
1.739E-03	2.740E-01	29.99	B403	1 2 2 2 2	
2.348E-03	3.700E-01	39.99	B403	1 2 2 2 2	
7.933E-04	1.250E-01	50	D071	1 2 0 0 2	
9.709E-04	1.530E-01	100	D071	1 2 0 0 2	
1.016E-03	1.600E-01	100	F300	1 0 0 0 2	

607. C₆H₄ClNO₂*m*-Chloronitrobenzene

1-Chloro-3-nitrobenzene

3-Chloronitrobenzene

m-Nitrochlorobenzene

RN: 121-73-3 MP (°C): 46.0

MW: 157.56 BP (°C): 236.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.732E-03	2.729E-01	20	E308	1 2 2 1 2	

608. C₆H₄ClNO₂*o*-Chloronitrobenzene

2-Nitrochlorobenzene

2-CNB

1-Chloro-2-nitrobenzene

RN: 88-73-3 MP (°C): 32

MW: 157.56 BP (°C): 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-03	2.280E-01	9.99	B403	1 2 2 2 2	
2.133E-03	3.360E-01	19.99	B403	1 2 2 2 2	
2.800E-03	4.412E-01	20	E308	1 2 2 1 2	
<1.27E-03	<2.00E-01	25	B019	1 0 1 2 0	
3.470E-03	5.467E-01	25	G090	2 2 1 1 1	
3.199E-03	5.040E-01	29.99	B403	1 2 2 2 2	
4.271E-03	6.730E-01	39.99	B403	1 2 2 2 2	

609. C₆H₄Cl₂

1,2-Dichlorobenzene

o-Dichlorobenzene

RN: 95-50-1 MP (°C): -17

MW: 147.00 BP (°C): 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.047E-04	1.330E-01	3.5	C094	1 0 0 0 2	
1.007E-03	1.480E-01	20	C094	1 0 0 0 2	
9.114E-04	1.340E-01	20	K056	1 0 2 2 2	
9.550E-04	1.404E-01	20	K337	1 0 0 0 2	
6.607E-04	9.713E-02	22	K305	1 0 1 1 2	
<1.36E-03	<2.00E-01	25	B019	1 0 1 2 0	
1.060E-03	1.558E-01	25	B173	2 0 2 2 2	
9.864E-04	1.450E-01	25	B185	0 0 0 0 0	
9.319E-04	1.370E-01	25	B304	2 0 2 2 2	
8.000E-04	1.176E-01	25	B317	0 0 0 0 0	
1.047E-03	1.539E-01	25	C113	1 0 2 2 2	
9.864E-04	1.450E-01	25	K056	1 0 2 2 2	
1.156E-03	1.700E-01	25	L319	1 0 2 1 1	
6.280E-04	9.232E-02	25	M342	1 0 1 1 2	
1.163E-03	1.710E-01	30	K056	1 0 2 2 2	

(continued)

609. C₆H₄Cl₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.016E-03	1.494E-01	30	M300	1 1 2 2 2	
9.680E-04	1.423E-01	30	M311	1 1 2 2 2	
1.245E-03	1.830E-01	35	K056	1 0 2 2 2	
1.320E-03	1.940E-01	40	K056	1 0 2 2 2	
1.381E-03	2.030E-01	45	K056	1 0 2 2 2	
1.517E-03	2.230E-01	55	K056	1 0 2 2 2	
1.578E-03	2.320E-01	60	K056	1 0 2 2 2	
1.060E+03	1.558E+05	ns	A096	0 0 0 0 2	<i>sic</i>
6.280E-04	9.232E-02	ns	M308	0 0 1 1 2	

610. C₆H₄Cl₂

1,3-Dichlorobenzene

m-Dichlorobenzene

RN: 541-73-1 MP (°C): -24
 MW: 147.00 BP (°C): 172–173

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.551E-04	1.110E-01	20	K056	1 0 2 2 2	
7.943E-04	1.168E-01	20	K337	1 0 0 0 2	
4.677E-04	6.876E-02	22	K305	1 0 1 1 2	
9.080E-04	1.335E-01	25	B173	2 0 2 2 2	
9.728E-04	1.430E-01	25	B304	2 1 2 1 2	
8.300E-04	1.220E-01	25	B317	0 0 0 0 0	
9.120E-04	1.341E-01	25	C113	1 0 2 2 2	
8.367E-04	1.230E-01	25	K056	1 0 2 2 2	
8.470E-04	1.245E-01	25	M342	1 0 1 1 2	
9.523E-04	1.400E-01	30	K056	1 0 2 2 2	
8.537E-04	1.255E-01	30	M300	1 1 2 2 2	
8.537E-04	1.255E-01	30	M311	1 1 2 2 2	
1.020E-03	1.500E-01	35	K056	1 0 2 2 2	
1.136E-03	1.670E-01	40	K056	1 0 2 2 2	
1.204E-03	1.770E-01	45	K056	1 0 2 2 2	
1.333E-03	1.960E-01	55	K056	1 0 2 2 2	
1.367E-03	2.010E-01	60	K056	1 0 2 2 2	
9.080E+02	1.335E+05	ns	A096	0 0 0 0 2	<i>sic</i>
8.470E-04	1.245E-01	ns	M308	0 0 1 1 2	

611. C₆H₄Cl₂

1,4-Dichlorobenzene

p-Dichlorobenzene

RN: 106-46-7 MP (°C): 53.1
 MW: 147.00 BP (°C): 173.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.680E-04	6.880E-02	20	K056	1 2 2 1 2	average of 4
3.020E-04	4.439E-02	20	K337	1 0 0 0 2	
2.252E-04	3.310E-02	20	T301	1 2 2 2 2	

(continued)

611. C₆H₄Cl₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-04	4.868E-02	22	K305	1 0 1 1 2	
5.292E-04	7.780E-02	22.20	W003	2 2 2 2 2	average of 2
5.673E-04	8.340E-02	24.60	W003	2 2 2 2 2	average of 3
5.170E-04	7.600E-02	25	A003	1 0 1 2 1	
5.928E-04	8.715E-02	25	A058	1 1 1 1 2	
<3.40E-03	<5.00E-01	25	B019	1 0 1 2 0	
5.020E-04	7.380E-02	25	B173	2 0 2 2 2	
4.442E-04	6.530E-02	25	B304	2 0 2 2 2	
5.270E-04	7.747E-02	25	B317	0 0 0 0 0	
3.990E-04	5.865E-02	25	C316	0 0 0 0 0	0.1M NaCl
5.374E-04	7.900E-02	25	F071	1 1 2 1 1	
5.374E-04	7.900E-02	25	H080	1 0 0 0 1	
5.381E-04	7.910E-02	25	K056	1 2 2 2 2	average of 2
5.646E-04	8.300E-02	25	M040	1 0 0 1 1	
5.442E-04	8.000E-02	25	M161	1 0 0 0 1	
2.100E-04	3.087E-02	25	M342	1 0 1 1 2	
6.932E-05	1.019E-02	25	N311	1 0 1 1 2	
4.100E-04	6.027E-02	25.2	T428	0 0 0 0 0	
5.898E-04	8.670E-02	25.50	W003	2 2 2 2 2	average of 2
5.238E-04	7.699E-02	30	G029	1 0 2 2 1	
6.347E-04	9.330E-02	30	K056	1 2 2 2 2	
6.267E-04	9.213E-02	30	M300	1 1 2 2 2	
6.422E-04	9.440E-02	30	M311	1 1 2 2 2	
6.299E-04	9.260E-02	30.00	W003	2 2 2 2 2	average of 2
6.939E-04	1.020E-01	34.50	W003	2 2 2 2 2	average of 3
5.646E-04	8.300E-02	35	K056	1 2 2 2 2	
8.231E-04	1.210E-01	38.40	W003	2 2 2 2 2	
6.857E-04	1.008E-01	40	K056	1 2 2 2 2	average of 2
8.292E-04	1.219E-01	45	K056	1 2 2 2 2	average of 2
1.082E-03	1.590E-01	47.50	W003	2 2 2 2 2	
1.184E-03	1.740E-01	50.10	W003	2 2 2 2 2	average of 2
1.061E-03	1.560E-01	55	K056	1 2 2 2 2	
1.429E-03	2.100E-01	59.20	W003	2 2 2 2 2	
1.109E-03	1.630E-01	60	K056	1 2 2 2 2	
1.483E-03	2.180E-01	60.70	W003	2 2 2 2 2	average of 2
1.565E-03	2.300E-01	65.10	W003	2 2 2 2 2	average of 3
1.612E-03	2.370E-01	65.20	W003	2 2 2 2 2	average of 3
1.912E-03	2.810E-01	73.40	W003	2 2 2 2 2	
2.100E-04	3.087E-02	ns	M308	0 0 1 1 2	
5.374E-04	7.900E-02	ns	M344	0 0 0 0 1	
5.034E-04	7.400E-02	rt	S314	0 0 2 1 1	

612. C₆H₄Cl₂N₂O₂

Dicloran

RN: 99-30-9 MP (°C): 195
 MW: 207.02 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-05	6.252E-03	ns	R424	0 0 0 0 0	
3.020E-05	6.252E-03	ns	R427	0 0 0 0 0	

613. C₆H₄Cl₂O

2,4-Dichlorophenol

2,4-Dichlor-phenol

RN: 120-83-2**MP (°C):** 45**MW:** 163.00**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.390E-02	3.896E+00	15.3	A400	2 1 2 2 2	
2.748E-02	4.480E+00	19	D041	1 0 0 0 1	
~2.76E-02	~4.50E+00	20	F300	1 0 0 0 0	
2.748E-02	4.480E+00	20	N034	1 0 0 0 1	
3.403E-02	5.547E+00	25	M373	1 0 2 1 2	
3.052E-02	4.975E+00	25	R041	0 0 0 0 0	
3.385E-02	5.517E+00	25.2	A400	2 1 2 2 2	
1.748E-01	2.850E+01	34.6	A400	2 1 2 2 2	
2.754E-02	4.490E+00	ns	R427	0 0 0 0 0	

614. C₆H₄Cl₂O

3,5-Dichlorophenol

3,5-DCP

RN: 591-35-5**MP (°C):** 68**MW:** 163.00**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E-02	7.394E+00	25	M373	1 0 2 1 2	

615. C₆H₄Cl₂O

3,4-Dichlorophenol

4,5-Dichlorophenol

3,4-DCP

RN: 95-77-2**MP (°C):** 67**MW:** 163.00**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.678E-02	9.256E+00	25	M373	1 0 2 1 2	

616. C₆H₄Cl₂O

2,6-Dichlorophenol

2,6-DCP

RN: 87-65-0**MP (°C):** 66.5**MW:** 163.00**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-02	2.625E+00	25	M373	1 0 2 1 2	

617. C₆H₄Cl₂O

2,3-Dichlorophenol

Phenol, 2,3-dichloro-

RN: 576-24-9 MP (°C): 59

MW: 163.00 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.040E-02	8.215E+00	25	M373	1 0 2 1 2	

618. C₆H₄Cl₂O

2,5-Dichlorophenol

2,5-Dichlor-phenol

RN: 583-78-8 MP (°C):

MW: 163.00 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-02	6.194E+00	25	B316	0 0 0 0 0	

619. C₆H₄FI

1-Fluoro-4-iodobenzene

4-Fluoro-1-iodobenzene

p-Iodofluorobenzene*p*-Fluoroiodobenzene*p*-Fluorophenyl iodide

RN: 352-34-1 MP (°C): -27

MW: 222.00 BP (°C): 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.499E-04	1.665E-01	25	B349	2 0 2 0 2	

620. C₆H₄I₂

1,4-Diiodobenzene

p-Diiodobenzene

4-Iodophenyl iodide

RN: 624-38-4 MP (°C): 131

MW: 329.91 BP (°C): 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.244E-06	1.400E-03	25	A003	1 2 1 2 1	<i>sic</i>
3.100E-02	1.023E+01	25	C316	0 0 0 0 0	0.1M NaCl

621. C₆H₄N₂O₄*p*-Dinitrobenzene

1,4-Dinitrobenzene

RN: 100-25-4

MP (°C): 173

MW: 168.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.759E-04	8.000E-02	20	F300	1 0 0 0 0	
2.350E-04	3.951E-02	25	C316	0 0 0 0 0	0.1M NaCl
4.090E-04	6.876E-02	25	I334	2 2 2 1 2	
3.676E-04	6.180E-02	25	L008	2 2 2 1 2	average of 2
6.170E-04	1.037E-01	35	H077	2 2 2 2 2	
1.130E-02	1.900E+00	100	F300	1 0 0 0 1	

622. C₆H₄N₂O₄*m*-Dinitrobenzene

1,3-Dinitrobenzene

RN: 99-65-0

MP (°C): 89.5

MW: 168.11

BP (°C): 301.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.045E-04	6.800E-02	13	D070	1 2 0 0 1	
4.164E-04	7.000E-02	13	F300	1 0 0 0 0	
3.420E-03	5.749E-01	25	I334	2 2 2 1 2	
3.169E-03	5.328E-01	25	L008	2 2 2 1 2	average of 2
5.116E-03	8.600E-01	25.04	V013	2 2 2 2 2	
3.867E-03	6.500E-01	30	F300	1 0 0 0 1	
3.888E-03	6.536E-01	30	G029	1 0 2 2 2	
4.670E-03	7.851E-01	35	H077	2 2 2 2 2	
2.789E-03	4.688E-01	50	D070	1 2 0 0 2	
1.134E-02	1.906E+00	100	D070	1 2 0 0 2	
1.547E-02	2.600E+00	100	F300	1 0 0 0 1	
2.973E-03	4.998E-01	rt	D021	0 0 1 1 0	

623. C₆H₄N₂O₄*o*-Dinitrobenzene

1,2-Dinitrobenzene

RN: 528-29-0

MP (°C): 118

MW: 168.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.328E-04	1.400E-01	20	F300	1 0 0 0 1	
7.910E-04	1.330E-01	25	I334	2 2 2 1 2	
7.418E-04	1.247E-01	25	L008	2 2 2 1 2	average of 3

624. C₆H₄N₂O₅

3,5-Dinitrophenol

Phenol, θ-dinitro-

RN: 586-11-8

MP (°C):

MW: 184.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.288E-02	1.342E+01	51.6	S117	1 2 1 1 2	solid hydrate
2.373E+00	4.370E+02	54.1	S117	1 2 1 1 2	anhydrate
2.407E+00	4.431E+02	54.5	S117	1 2 1 1 2	anhydrate
2.442E+00	4.496E+02	55.5	S117	1 2 1 1 2	anhydrate
2.474E+00	4.555E+02	57.9	S117	1 2 1 1 2	anhydrate
2.516E+00	4.633E+02	61.9	S117	1 2 1 1 2	anhydrate
2.583E+00	4.756E+02	69.9	S117	1 2 1 1 2	anhydrate
2.617E+00	4.819E+02	81.3	S117	1 2 1 1 2	anhydrate
5.308E-01	9.772E+01	109.3	S117	1 0 1 1 2	
1.253E+00	2.307E+02	124.6	S117	1 0 1 1 2	

625. C₆H₄N₂O₅

2,6-Dinitrophenol

β-Dinitrophenol

RN: 573-56-8

MP (°C):

MW: 184.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-03	3.149E-01	15	D080	1 2 0 0 2	unit assumed
1.629E-03	3.000E-01	15	F300	1 0 0 0 0	
2.805E-02	5.164E+00	50	D080	1 2 0 0 2	unit assumed
6.547E-02	1.205E+01	100	D080	1 2 0 0 2	unit assumed
6.518E-02	1.200E+01	100	F300	1 0 0 0 1	

626. C₆H₄N₂O₅

2,4-Dinitrophenol

α-Dinitrophenol

Aldifen

Fenoxy carbon N

RN: 51-28-5

MP (°C): 107.5

MW: 184.11

BP (°C): 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.097E-03	2.020E-01	12.5	D069	1 2 0 0 2	
1.086E-03	2.000E-01	12.50	F300	1 0 0 0 0	
1.629E-03	2.999E-01	15	D079	1 2 0 0 1	
2.254E-03	4.150E-01	15.1	A400	2 1 2 2 2	
3.025E-02	5.569E+00	18	D041	1 0 0 0 1	
2.800E-02	5.155E+00	20	K301	2 2 1 1 1	
2.524E-03	4.647E-01	25	H085	2 0 2 1 2	

(continued)

626. C₆H₄N₂O₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.467E-03	2.700E-01	25	P037	2 0 1 1 2	
3.753E-03	6.910E-01	25.0	A400	2 1 2 2 2	
1.901E-01	3.500E+01	35.0	A400	2 1 2 2 2	
4.356E-03	8.020E-01	50	D069	1 2 0 0 2	
9.504E-04	1.750E-01	50	D079	1 2 0 0 2	
7.431E-03	1.368E+00	54.50	E032	1 2 1 2 2	
1.192E-02	2.195E+00	67.60	E032	1 2 1 2 2	
1.630E-02	3.001E+00	75.80	E032	1 2 1 2 2	
3.414E-02	6.286E+00	85	D069	1 2 0 0 2	
3.170E-02	5.836E+00	87.40	E032	1 2 1 2 2	
4.845E-02	8.920E+00	92.40	E032	1 2 1 2 2	
6.547E-02	1.205E+01	96.20	E032	1 2 1 2 2	
7.163E-02	1.319E+01	100	D069	1 2 0 0 2	
8.964E-02	1.650E+01	100	D079	1 2 0 0 2	
7.061E-02	1.300E+01	100	F300	1 0 0 0 1	
2.444E-01	4.500E+01	h	F300	0 0 0 0 1	
2.702E-02	4.975E+00	ns	M061	0 0 0 0 0	

627. C₆H₄N₂O₆

2,4-Dinitroresorcinol

2,4-Dinitro-1,3-benzenediol

RN: 519-44-8 MP (°C):
 MW: 200.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.129E-02	6.261E+00	57.70	E032	1 2 1 2 2	
4.801E-02	9.607E+00	66.60	E032	1 2 1 2 2	
7.434E-02	1.488E+01	69.50	E032	1 2 1 2 2	
9.895E-02	1.980E+01	76.50	E032	1 2 1 2 2	
1.690E-01	3.382E+01	84.70	E032	1 2 1 2 2	
2.380E-01	4.762E+01	90.00	E032	1 2 1 2 2	
3.495E-01	6.994E+01	93.00	E032	1 2 1 2 2	

628. C₆H₄N₂O₆

4,6-Dinitroresorcinol

4,6-Dinitro-1,3-benzenediol

RN: 616-74-0 MP (°C):
 MW: 200.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	3.998E-01	77.00	E032	1 2 1 2 2	
3.995E-03	7.994E-01	90.50	E032	1 2 1 2 2	
4.992E-03	9.990E-01	96.30	E032	1 2 1 2 2	

629. C₆H₄N₄

Pteridine

1,3,5,8-Tetraazanaphthalene

Azinepurine

Pyrimido[4,5-b]pyrazine

Pyrazino[2,3-d]pyrimidine

RN: 91-18-9**MP (°C):** 138**MW:** 132.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.461E-01	1.250E+02	20	A020	1 2 0 0 1	
9.461E-01	1.250E+02	20	B050	1 0 0 0 0	
9.230E-01	1.220E+02	22.5	A085	1 2 0 0 0	
3.784E+00	5.000E+02	100	B050	1 0 0 0 0	

630. C₆H₄N₄O

4-Hydroxypteridine

4-Pteridinol

RN: 700-47-0**MP (°C):****MW:** 148.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.359E-02	4.975E+00	20	A020	1 2 0 0 1	
3.359E-02	4.975E+00	20	B050	1 0 0 0 0	
3.359E-02	4.975E+00	22.5	A085	1 2 0 0 0	
2.250E-01	3.333E+01	100	B050	1 0 0 0 0	

631. C₆H₄N₄O

6-Hydroxypteridine

6-Pteridinol

RN: 2432-26-0**MP (°C):****MW:** 148.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.928E-03	2.856E-01	20	A020	1 2 0 0 1	
1.928E-03	2.856E-01	20	B050	1 0 0 0 0	
2.923E-02	4.329E+00	100	B050	1 0 0 0 0	

632. C₆H₄N₄O

7-Hydroxypteridine

7-Pteridinol

RN: 2432-27-1**MP (°C):****MW:** 148.12**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.493E-03	1.110E+00	20	B050	1 0 0 0 0	
8.768E-02	1.299E+01	100	B050	1 0 0 0 0	

633. C₆H₄N₄O

2-Hydroxypteridine

2-Pteridinol

RN: 25911-76-6 **MP (°C):** 240
MW: 148.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.123E-02	1.664E+00	20	A020	1 2 0 0 1	
1.123E-02	1.664E+00	20	B050	1 0 0 0 0	
1.123E-02	1.664E+00	22.5	A085	1 2 0 0 0	
1.324E-01	1.961E+01	100	B050	1 0 0 0 0	

634. C₆H₄N₄O₂

2,4-Dihydroxypteridine

2:4-Dihydroxypteridine

Lumazine

RN: 487-21-8 **MP (°C):** 348.5
MW: 164.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.607E-03	1.248E+00	20	B050	1 0 0 0 0	
7.607E-03	1.248E+00	22.5	A085	1 2 0 0 0	
5.035E-02	8.264E+00	100	B050	1 0 0 0 0	

635. C₆H₄N₄O₂

2,7-Dihydroxypteridine

2:7-Dihydroxypteridine

RN: 65882-62-4 **MP (°C):**
MW: 164.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.033E-02	9.901E+00	100	A020	1 2 0 0 0	

636. C₆H₄N₄O₂

4,6-Dihydroxypteridine

4:6-Dihydroxypteridine

RN: 16310-36-4 **MP (°C):**
MW: 164.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.108E-03	1.818E-01	20	A020	1 2 0 0 1	
1.218E-03	2.000E-01	20	B050	1 0 0 0 0	
2.024E-02	3.322E+00	100	B050	1 0 0 0 0	

637. C₆H₄N₄O₂

4,7-Dihydroxypteridine

4:7-Dihydroxypteridine

6,7-Dihydroxypteridine

6:7-Dihydroxypteridine

RN: 33669-70-4 **MP (°C):****MW:** 164.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.030E-03	3.332E-01	20	A020	1 2 0 0 1	
1.523E-03	2.499E-01	20	A020	1 2 0 0 1	
2.030E-03	3.332E-01	20	B050	1 0 0 0 0	
1.523E-03	2.499E-01	20	B050	1 0 0 0 0	
2.094E-02	3.436E+00	100	B050	1 0 0 0 0	
1.014E-02	1.664E+00	100	B050	1 0 0 0 0	

638. C₆H₄N₄O₂

2,6-Dihydroxypteridine

2:6-Dihydroxypteridine

RN: 89324-38-9 **MP (°C):****MW:** 164.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.354E-03	2.222E-01	100	A020	1 2 0 0 1	

639. C₆H₄N₄O₃

2,4,7-Trihydroxypteridine

2:4:7-Trihydroxypteridine

RN: 2577-38-0 **MP (°C):****MW:** 180.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.626E-04	8.333E-02	20	A020	1 2 0 1 1	
4.626E-04	8.333E-02	20	B050	1 0 0 0 0	
3.963E-03	7.138E-01	100	A020	1 2 0 0 1	
3.963E-03	7.138E-01	100	B050	1 0 0 0 0	

640. C₆H₄N₄O₃

4,6,7-Trihydroxypteridine

4:6:7-Trihydroxypteridine

RN: 58947-88-9 **MP (°C):****MW:** 180.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E-04	3.704E-02	20	A020	1 2 0 0 1	
2.056E-04	3.704E-02	20	B050	1 0 0 0 0	
7.930E-04	1.428E-01	100	B050	1 0 0 0 0	

641. C₆H₄N₄O₄

2,4,6,7-Tetrahydroxypteridine

2,4,6-Trihydroxypteridine

2:4:6-Trihydroxypteridine

RN: 2817-14-3 **MP (°C):****MW:** 196.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.791E-05	1.724E-02	20	A020	1 2 0 1 1	
6.889E-04	1.351E-01	20	B050	1 0 0 0 0	
8.791E-05	1.724E-02	20	B050	1 0 0 0 0	
1.272E-02	2.494E+00	100	A020	1 2 0 0 0	
7.283E-04	1.428E-01	100	A020	1 2 0 0 0	
1.272E-02	2.494E+00	100	B050	1 0 0 0 0	

642. C₆H₄N₄O₆

Picramine

2,4,6-Trinitroaniline

1-Amino-2,4,6-trinitrobenzene

MATB

RN: 489-98-5 **MP (°C):** 192**MW:** 228.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.710E-05	1.987E-02	25	B335	1 2 0 0 1	

643. C₆H₄N₄S

4-Mercaptopteridine

4-Pteridinethiol

4(1H)-Pteridinethione

Pteridine-4-thiol

RN: 65882-61-3 **MP (°C):** 176dec**MW:** 164.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.691E-03	2.777E-01	22.5	A085	1 2 0 0 0	

644. C₆H₄N₄S

2-Mercaptopteridine

2-Pteridinethiol

2(1H)-Pteridinethione

RN: 16878-76-5 **MP (°C):** 205**MW:** 164.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.347E-03	7.138E-01	22.5	A085	1 2 0 0 0	

645. C₆H₄N₄S

7-Mercaptopteridine

7-Pteridinethiol

7(1H)-Pteridinethione

RN: 36653-71-1 **MP (°C):**
MW: 164.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.964E-03	3.225E-01	20	A083	1 2 0 0 0	
6.760E-03	1.110E+00	100	A083	1 2 0 0 0	

646. C₆H₄O₂

Quinone

1,4-Benzooquinone

Benzochinhydrone

p-Quinone

RN: 106-51-4 **MP (°C):** 115.7
MW: 108.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-02	9.329E+00	11.85	L064	2 2 2 1 2	0.01N HCl
1.013E-01	1.095E+01	17.70	L065	1 0 0 0 2	0.01N HCl
1.021E-01	1.104E+01	17.90	L065	1 0 0 0 2	0.01N HCl
1.030E-01	1.113E+01	17.95	L065	1 0 0 0 2	0.01N HCl
1.030E-01	1.113E+01	18	L064	2 2 2 1 2	0.01N HCl
1.580E-02	1.708E+00	20	B113	1 2 2 1 2	
1.233E-01	1.333E+01	23.85	L064	2 2 2 1 2	0.01N HCl
1.295E-01	1.400E+01	24	F300	1 0 0 0 1	
1.266E-01	1.369E+01	25	G033	1 0 1 1 2	
1.397E-01	1.510E+01	25	K033	1 0 0 1 2	

647. C₆H₄O₅

2,5-Dicarboxyfuran

Furan-dicarbon-saeure-(2,5)

RN: 3238-40-2 **MP (°C):**
MW: 156.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.406E-03	1.000E+00	18	F300	1 0 0 0 0	

648. C₆H₄O₅

2-Carboxy-5-hydroxy-4-pyrone

Komensaeure

Komenic acid

RN: 499-78-5**MP (°C):****MW:** 156.10**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.267E-02	5.100E+00	25	F300	1 0 0 0 1	
3.921E-01	6.120E+01	100	F300	1 0 0 0 2	

649. C₆H₅Br

Bromobenzene

Phenyl bromide

Monobromobenzene

RN: 108-86-1**MP (°C):** -30**MW:** 157.02**BP (°C):** 156.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.611E-03	4.100E-01	25	A003	1 2 1 2 1	
2.620E-03	4.114E-01	25	W300	2 2 2 2 2	
2.840E-03	4.460E-01	30	F071	1 1 2 1 2	
2.966E-03	4.658E-01	30	G029	1 0 2 2 2	
2.840E-03	4.460E-01	30	H080	1 0 0 0 2	
2.102E-03	3.300E-01	30	M311	1 1 2 2 2	
2.799E-03	4.395E-01	30	V009	1 0 0 0 1	
2.920E-03	4.585E-01	35	H077	2 2 2 2 2	
5.110E-04	8.024E-02	ns	D348	0 0 0 0 0	
2.615E-03	4.106E-01	ns	M344	0 0 0 0 2	

650. C₆H₅BrO*p*-Bromophenol

4-Bromophenol

RN: 106-41-2**MP (°C):** 66**MW:** 173.02**BP (°C):** 236

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.053E-02	1.393E+01	20	R087	0 0 0 0 0	0.15M NaCl
8.542E-02	1.478E+01	25	R041	0 0 0 0 0	
8.128E-02	1.406E+01	ns	R424	0 0 0 0 0	

651. C₆H₅BrO₃S*p*-Bromobenzenesulfonic acid

4-Bromobenzenesulfonic acid

RN: 138-36-3 MP (°C):

MW: 237.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.079E+00	4.929E+02	82.3	T023	1 2 2 1 2	
2.088E+00	4.949E+02	89.6	T023	1 2 2 1 2	
2.093E+00	4.961E+02	93.1	T023	1 2 2 1 2	
2.097E+00	4.972E+02	97.6	T023	1 2 2 1 2	

652. C₆H₅BrO₃S.H₂O*p*-Bromobenzenesulfonic acid (monohydrate)

RN: 138-36-3 MP (°C):

MW: 255.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.799E+00	4.588E+02	43.8	T023	1 2 2 1 2	
1.821E+00	4.644E+02	60.2	T023	1 2 2 1 2	
1.586E+00	4.045E+02	71.2	T023	1 2 2 1 2	
1.924E+00	4.909E+02	76.6	T023	1 2 2 1 2	
1.922E+00	4.903E+02	78.5	T023	1 2 2 1 2	
1.855E+00	4.731E+02	80.3	T023	1 2 2 1 2	
1.868E+00	4.766E+02	86.2	T023	1 2 2 1 2	
1.907E+00	4.865E+02	87.2	T023	1 2 2 1 2	
1.889E+00	4.818E+02	90.2	T023	1 2 2 1 2	

653. C₆H₅BrO₃S.2.5H₂O*p*-Bromobenzenesulfonic acid (2.5 hydrate)

RN: 138-36-3 MP (°C):

MW: 282.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.375E+00	3.880E+02	-21.0	T023	1 2 2 1 2	
1.409E+00	3.975E+02	-10.5	T023	1 2 2 1 2	
1.495E+00	4.219E+02	12.5	T023	1 2 2 1 2	
1.522E+00	4.294E+02	19.9	T023	1 2 2 1 2	
1.566E+00	4.418E+02	27.6	T023	1 2 2 1 2	
1.613E+00	4.550E+02	34.6	T023	1 2 2 1 2	
1.447E+00	4.081E+02	.0	T023	1 2 2 1 2	

654. C₆H₅Cl

Chlorobenzene

IP Carrier T 40

Phenyl chloride

Tetrosin SP

Monochlorobenzene

MCB

RN: 108-90-7 **MP (°C):** -45
MW: 112.56 **BP (°C):** 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-03	4.802E-01	20	K337	1 0 0 0 2	
4.440E-03	4.998E-01	20	M312	1 0 0 0 2	
4.742E-03	5.337E-01	21	C024	2 1 1 2 2	
4.442E-03	5.000E-01	25	A003	1 2 1 2 1	
4.191E-03	4.717E-01	25	A058	1 1 1 1 2	
<1.78E-03	<2.00E-01	25	B019	1 0 1 2 0	
4.460E-03	5.020E-01	25	B304	2 0 2 2 2	
4.300E-03	4.840E-01	25	B317	0 0 0 0 0	
3.108E-03	3.499E-01	25	L319	1 0 2 1 1	
2.620E-03	2.949E-01	25	M342	1 0 1 1 2	
3.540E-02	3.984E+00	25	N309	1 0 0 0 1	<i>sic</i>
3.780E-03	4.255E-01	25	S359	2 1 2 2 2	
4.430E-03	4.986E-01	25	W300	2 2 2 2 2	
9.762E-03	1.099E+00	25.50	O005	2 0 2 2 1	<i>sic</i>
8.884E-04	1.000E-01	26.70	L095	2 2 1 1 2	
3.980E-03	4.480E-01	30	F071	1 1 2 1 2	
4.353E-03	4.900E-01	30	F300	1 0 0 0 1	
4.333E-03	4.878E-01	30	G029	1 0 2 2 2	
3.980E-03	4.480E-01	30	H080	1 0 0 0 2	
4.000E-03	4.502E-01	30	H332	2 2 2 2 0	
4.351E-03	4.898E-01	30	K065	2 0 2 1 2	
4.211E-03	4.740E-01	30	M300	1 1 2 2 2	
4.211E-03	4.740E-01	30	M311	1 1 2 2 2	
4.298E-03	4.838E-01	30	V009	1 0 0 0 1	
6.259E-03	7.045E-01	40	K065	2 0 2 1 2	
3.560E-03	4.007E-01	45	N043	1 0 2 2 2	
8.521E-03	9.591E-01	50	K065	2 0 2 1 2	
9.762E-03	1.099E+00	60	K065	2 0 2 1 2	
1.424E-02	1.602E+00	70	K065	2 0 2 1 2	
1.601E-02	1.802E+00	80	K065	2 0 2 1 2	
2.216E-02	2.494E+00	90	K065	2 0 2 1 2	
4.185E-03	4.711E-01	ns	H123	0 0 0 0 0	
2.620E-03	2.949E-01	ns	M308	0 0 1 1 2	
4.193E-03	4.720E-01	ns	M344	0 0 0 0 2	

655. C₆H₅CIN₂O₄S

4-Chloro-3-nitro-benzenesulfonamide
Benzenesulfonamide, 4-chloro-3-nitro-

RN: 97-09-6 **MP (°C):**
MW: 236.63 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-04	2.248E-01	15	K024	1 2 1 1 2	

656. C₆H₅ClO

m-Chlorophenol
3-Chlorophenol
Chlorophenate
3-Hydroxychlorobenzene

RN: 108-43-0 **MP (°C):** 33
MW: 128.56 **BP (°C):** 214

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.945E-01	2.500E+01	20	F300	1 0 0 0 1	
1.919E-01	2.468E+01	20	N034	1 0 0 0 2	
1.726E-01	2.219E+01	25	M373	1 0 2 1 2	
1.995E-01	2.565E+01	ns	R427	0 0 0 0 0	

657. C₆H₅ClO

p-Chlorophenol
4-Chloro-phenol-
Parachlorophenol
4-Hydroxychlorobenzene
4-Chlorophenol
4-Hydroxychlorobenzene

RN: 106-48-9 **MP (°C):** 43.2
MW: 128.56 **BP (°C):** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.815E-01	2.334E+01	15.1	A400	2 1 2 2 2	
2.022E-01	2.600E+01	20	F300	1 0 0 0 1	
1.022E-01	1.314E+01	20	H301	0 0 0 0 0	
1.993E-01	2.563E+01	20	N034	1 0 0 0 2	
1.839E-01	2.364E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.100E-01	2.700E+01	25	B316	0 0 0 0 0	
2.053E-01	2.639E+01	25	M373	1 0 2 1 2	
1.823E-01	2.344E+01	25	R041	0 0 0 0 0	
1.987E-01	2.554E+01	25.2	A400	2 1 2 2 2	
1.867E-01	2.401E+01	34.5	A400	2 1 2 2 2	
4.898E+00	6.297E+02	ns	R427	0 0 0 0 0	

658. C₆H₅ClO

o-Chlorophenol

2-Chlorophenol

RN: 95-57-8

MP (°C): 9.3

MW: 128.56

BP (°C): 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.621E-01	2.084E+01	15.4	A400	2 1 2 2 2	
1.763E-01	2.266E+01	24.6	A400	2 1 2 2 2	
8.830E-02	1.135E+01	25	B173	2 0 2 2 2	
1.809E-01	2.326E+01	25	M373	1 0 2 1 2	
1.674E-01	2.153E+01	25	R041	0 0 0 0 0	
2.097E-01	2.695E+01	ns	N034	0 0 0 0 2	

659. C₆H₅ClO₃S*p*-Chlorobenzenesulfonic acid

4-Chlor-benzolsulfosaeure

RN: 98-66-8

MP (°C): 67

MW: 192.62

BP (°C): 148

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.583E+00	4.975E+02	59.0	T023	1 2 2 1 2	
2.590E+00	4.988E+02	62.4	T023	1 2 2 1 2	

660. C₆H₅ClO₃S.2.5H₂O*p*-Chlorobenzenesulfonic acid (2.5 hydrate)

RN: 98-66-8

MP (°C):

MW: 237.66

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.519E+00	3.609E+02	-26.0	T023	1 2 2 1 2	
1.553E+00	3.690E+02	-20.0	T023	1 2 2 1 2	
1.606E+00	3.816E+02	-11.0	T023	1 2 2 1 2	
1.653E+00	3.929E+02	-2.2	T023	1 2 2 1 2	
1.723E+00	4.095E+02	10.6	T023	1 2 2 1 2	
1.784E+00	4.240E+02	22.9	T023	1 2 2 1 2	
1.817E+00	4.318E+02	27.6	T023	1 2 2 1 2	
1.854E+00	4.406E+02	30.8	T023	1 2 2 1 2	

661. C₆H₅Cl₂NO₂S

3,4-Dichloro-benzenesulfonamide

Benzenesulfonamide, 3,4-dichloro-

RN: 23815-28-3

MP (°C):

MW: 226.08

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-03	7.913E-01	15	K024	1 2 1 1 2	

662. C₆H₅Cl₂PS

Dichlorophenylphosphine sulfide
 Benzene phosphorus thiodichloride
 Phenylphosphonothioic dichloride
 Phenyl phosphorus thiodichloride
 DCPPS

RN: 3497-00-5 **MP (°C):**
MW: 211.05 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.211E-03	1.522E+00	23	W402	0 0 0 0 0	
2.597E-02	5.481E+00	32	W402	0 0 0 0 0	
4.676E-02	9.868E+00	40	W402	0 0 0 0 0	
7.060E-02	1.490E+01	50	W402	0 0 0 0 0	

663. C₆H₅F

Fluorobenzene

Fluorbenzol

RN: 462-06-6 **MP (°C):** -42
MW: 96.11 **BP (°C):** 85

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-02	1.550E+00	25	A003	1 2 1 2 2	
1.602E-02	1.540E+00	30	F071	1 1 2 1 2	
1.561E-02	1.500E+00	30	F300	1 0 0 0 1	
1.602E-02	1.540E+00	30	H080	1 0 0 0 2	
1.600E-02	1.538E+00	30	J036	0 0 0 0 0	
1.598E-02	1.535E+00	30	V009	1 0 0 0 2	
1.616E-02	1.553E+00	ns	M344	0 0 0 0 2	

664. C₆H₅FN₂O₃

3-Acetyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

3-Acetyl-5-fluorouracil

RN: 75410-15-0 **MP (°C):** 115–116
MW: 172.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.487E-01	4.280E+01	22	B321	0 0 0 0 0	pH 4.0
1.660E-01	2.857E+01	22	B416	2 2 1 2 1	

665. C₆H₅FN₂O₄

1-Methoxycarbonyl-5-fluorouracil

1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, methyl ester

RN: 71759-43-8 **MP (°C):**
MW: 188.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-01	2.330E+01	22	B332	1 1 0 0 1	pH 4.0

666. C₆H₅FO

2-Fluorophenol

2-Fluor-phenol

o-Fluorophenol**RN:** 367-12-4**MP (°C):** 16.1**MW:** 112.10**BP (°C):** 171.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-01	8.072E+01	25	P031	0 0 0 0 0	

667. C₆H₅FO*m*-Fluorophenol

3-Fluorophenol

RN: 372-20-3**MP (°C):** 13.7**MW:** 112.10**BP (°C):** 178

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-01	7.735E+01	25	P031	0 0 0 0 0	

668. C₆H₅FO*p*-Fluorophenol

4-Fluorophenol

RN: 371-41-5**MP (°C):** 46–48**MW:** 112.10**BP (°C):** 185–188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.671E-01	6.357E+01	20	R087	0 0 0 0 0	0.15M NaCl
7.200E-01	8.072E+01	25	P031	0 0 0 0 0	

669. C₆H₅FO₃S.H₂O*p*-Fluorobenzenesulfonic acid (monohydrate)**RN:** 368-88-7**MP (°C):****MW:** 194.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.243E+00	4.355E+02	22.1	T023	1 2 2 1 2	
2.263E+00	4.394E+02	35.4	T023	1 2 2 1 2	
2.549E+00	4.950E+02	41.4	T023	1 2 2 1 2	
2.306E+00	4.477E+02	54.2	T023	1 2 2 1 2	
2.539E+00	4.930E+02	54.3	T023	1 2 2 1 2	
2.356E+00	4.575E+02	71.2	T023	1 2 2 1 2	
2.509E+00	4.872E+02	74.5	T023	1 2 2 1 2	
2.392E+00	4.644E+02	80.0	T023	1 2 2 1 2	
2.496E+00	4.847E+02	81.0	T023	1 2 2 1 2	
2.463E+00	4.782E+02	85.2	T023	1 2 2 1 2	
2.440E+00	4.739E+02	85.5	T023	1 2 2 1 2	

670. C₆H₅FO₃S.2.5H₂O*p*-Fluorobenzenesulfonic acid (2.5 hydrate)

RN: 368-88-7 **MP (°C):**
MW: 221.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.848E+00	4.088E+02	-15.5	T023	1 2 2 1 2	
1.880E+00	4.160E+02	-3.9	T023	1 2 2 1 2	
1.893E+00	4.187E+02	1.0	T023	1 2 2 1 2	
1.923E+00	4.254E+02	10.1	T023	1 2 2 1 2	
1.966E+00	4.349E+02	21.3	T023	1 2 2 1 2	

671. C₆H₅FO₃S.3H₂O*p*-Fluorobenzenesulfonic acid (trihydrate)

RN: 368-88-7 **MP (°C):**
MW: 230.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.731E+00	3.985E+02	-22.5	T023	1 2 2 1 2	
1.704E+00	3.922E+02	-21.4	T023	1 2 2 1 2	
1.751E+00	4.032E+02	-19.5	T023	1 2 2 1 2	
1.760E+00	4.052E+02	-17.9	T023	1 2 2 1 2	
1.715E+00	3.949E+02	-18.5	T023	1 2 2 1 2	
1.751E+00	4.032E+02	-13.0	T023	1 2 2 1 2	
1.784E+00	4.108E+02	-7.4	T023	1 2 2 1 2	

672. C₆H₅FO₃S.4H₂O*p*-Fluorobenzenesulfonic acid (tetrahydrate)

RN: 368-88-7 **MP (°C):**
MW: 248.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E+00	3.648E+02	-38.0	T023	1 2 2 1 2	
1.484E+00	3.684E+02	-35.4	T023	1 2 2 1 2	
1.498E+00	3.719E+02	-34.4	T023	1 2 2 1 2	
1.519E+00	3.771E+02	-32.5	T023	1 2 2 1 2	
1.532E+00	3.803E+02	-30.5	T023	1 2 2 1 2	
1.580E+00	3.922E+02	-26.4	T023	1 2 2 1 2	
1.605E+00	3.985E+02	-24.0	T023	1 2 2 1 2	

673. C₆H₅I

Iodobenzene

RN: 591-50-4 **MP (°C):** -30
MW: 204.01 **BP (°C):** 188

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.823E-04	1.800E-01	25	A003	1 2 1 2 1	
9.840E-04	2.007E-01	25	M342	1 0 1 1 2	

(continued)

673. C₆H₅I (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-03	3.400E-01	30	F071	1 1 2 1 2	
1.667E-03	3.400E-01	30	F300	1 0 0 0 2	
1.667E-03	3.400E-01	30	H080	1 0 0 0 2	
1.667E-03	3.400E-01	30	M344	1 0 0 0 2	
1.699E-03	3.467E-01	30	V009	1 0 0 0 1	

674. C₆H₅IO*p*-Iodophenol

4-Iodophenol

RN: 540-38-5

MP (°C): 94

MW: 220.01

BP (°C): 138 at 5 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.285E-02	2.828E+00	20	R087	0 0 0 0 0	0.15M NaCl

675. C₆H₅NO₂

Nitrobenzene

Nitrobenzol

Benzene, nitro-

RN: 98-95-3

MP (°C): 6

MW: 123.11

BP (°C): 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	1.700E+00	6	V004	1 0 1 2 2	
1.438E-02	1.770E+00	9.99	B403	1 2 2 2 2	
1.443E-02	1.777E+00	15	G029	1 0 2 2 2	
1.568E-02	1.930E+00	19.99	B403	1 2 2 2 2	
1.549E-02	1.907E+00	20	B179	0 0 0 0 0	
1.543E-02	1.900E+00	20	F300	1 0 0 0 1	
1.600E-02	1.970E+00	20	P073	1 0 0 1 2	
1.543E-02	1.900E+00	22.5	G301	0 0 0 0 0	
1.568E-02	1.930E+00	25	A003	1 2 1 2 2	
1.700E-02	2.093E+00	25	B173	2 0 2 2 2	
1.580E-02	1.945E+00	25	H071	2 2 2 1 2	
1.600E-02	1.970E+00	25	H332	2 2 2 2 1	
1.560E-02	1.921E+00	25	I334	2 2 2 1 2	
1.560E-02	1.921E+00	25	I335	2 2 2 2 2	
1.543E-02	1.900E+00	25	M087	1 1 2 1 2	
1.457E-02	1.794E+00	25.04	V013	2 2 2 2 2	
1.446E-02	1.780E+00	26.70	L095	2 2 1 1 2	
1.673E-02	2.060E+00	29.99	B403	1 2 2 2 2	
1.662E-02	2.046E+00	30	G029	1 0 2 2 2	
1.673E-02	2.060E+00	30	V004	1 0 1 2 2	
1.667E-02	2.052E+00	30	V009	1 0 0 0 2	
1.835E-02	2.259E+00	35	H077	2 2 2 2 2	

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675. C₆H₅NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.787E-02	2.200E+00	39.99	B403	1 2 2 2 2	
2.144E-02	2.640E+00	50	V004	1 0 1 2 2	
2.193E-02	2.700E+00	55	F300	1 0 0 0 1	
2.534E-02	3.120E+00	60	V004	1 0 1 2 2	
2.700E-03	3.324E-01	ns	D348	0 0 0 0 0	

676. C₆H₅NO₂

Nicotinic acid

Niacin

RN: 59-67-6 MP (°C): 236
 MW: 123.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
1.208E-01	1.488E+01	1	H083	1 2 2 1 2	
2.679E-01	3.298E+01	16	C033	1 0 2 1 2	
1.358E-01	1.672E+01	20	D041	1 0 0 0 1	
1.436E-01	1.768E+01	20	H083	1 2 2 1 2	
1.381E-01	1.700E+01	20	M054	1 0 0 0 1	
3.652E-01	4.496E+01	28	C033	1 0 2 1 2	
2.595E-01	3.195E+01	42	H083	1 2 2 1 2	
3.735E-01	4.598E+01	60	H083	1 2 2 1 2	
5.604E-01	6.899E+01	80	H083	1 2 2 1 2	
6.809E-01	8.383E+01	88	H083	1 2 2 1 2	

677. C₆H₅NO₃*o*-Nitrophenol

2-Nitrophenol

RN: 88-75-5 MP (°C): 44
 MW: 139.11 BP (°C): 214

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
6.434E-03	8.950E-01	9.99	B403	1 2 2 2 2	
7.735E-03	1.076E+00	15.6	A400	2 1 2 2 2	
9.704E-03	1.350E+00	19.99	B403	1 2 2 2 2	
1.000E-02	1.391E+00	20	H306	1 0 1 2 1	
9.906E-03	1.378E+00	23.10	E032	1 2 1 2 2	
1.220E-02	1.697E+00	24.8	A400	2 1 2 2 2	
1.793E-02	2.494E+00	25	D006	1 2 0 1 2	
1.797E-02	2.500E+00	25	D059	1 2 1 1 1	
1.438E-02	2.000E+00	29.99	B403	1 2 2 2 2	
1.163E-02	1.617E+00	30.40	E032	1 2 1 2 2	
2.110E-02	2.935E+00	34.7	A400	2 1 2 2 2	
1.456E-02	2.026E+00	36.20	E032	1 2 1 2 2	
2.300E-02	3.200E+00	38.40	F300	1 0 0 0 1	
1.936E-02	2.693E+00	39.80	E032	1 2 1 2 2	

(continued)

677. C₆H₅NO₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.042E-02	2.840E+00	39.99	B403	1 2 2 2 2	
2.157E-02	3.000E+00	40	D059	1 2 1 1 0	
2.864E-02	3.984E+00	54.60	E032	1 2 1 2 1	
3.598E-02	5.005E+00	67.20	E032	1 2 1 2 2	
4.429E-02	6.162E+00	72.10	E032	1 2 1 2 2	
5.174E-02	7.198E+00	86.90	E032	1 2 1 2 2	
6.560E-02	9.126E+00	93.80	E032	1 2 1 2 2	
7.979E-02	1.110E+01	100	F300	1 0 0 0 2	

678. C₆H₅NO₃*p*-Nitrophenol

4-Nitrophenol

RN: 100-02-7

MP (°C): 113

MW: 139.11

BP (°C): 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.576E-02	4.975E+00	0	D006	1 2 0 1 1	
5.787E-02	8.050E+00	9.99	B403	1 2 2 2 2	
7.821E-02	1.088E+01	12.5	D006	1 2 0 1 1	
7.610E-02	1.059E+01	12.60	E032	1 2 1 2 2	
5.780E-02	8.040E+00	15	D069	1 2 0 0 2	
7.305E-02	1.016E+01	15.3	A400	2 1 2 2 2	
1.139E-01	1.584E+01	17.30	E032	1 2 1 2 2	
8.770E-02	1.220E+01	19.99	B403	1 2 2 2 2	
9.700E-02	1.349E+01	20	H306	1 0 1 2 1	
7.188E-02	9.999E+00	20	T301	1 2 2 2 2	
1.078E-01	1.500E+01	22.5	G301	0 0 0 0 0	
1.132E-01	1.575E+01	25	D006	1 2 0 1 1	
1.797E-01	2.500E+01	25	D059	1 2 1 1 1	
8.411E-02	1.170E+01	25	F300	1 0 0 0 2	
9.925E-02	1.381E+01	25	R041	0 0 0 0 0	
1.121E-01	1.560E+01	25.0	A400	2 1 2 2 2	
1.430E-01	1.990E+01	26.60	E032	1 2 1 2 2	
1.794E-01	2.496E+01	27.70	E032	1 2 1 2 2	
2.101E-01	2.922E+01	29.60	E032	1 2 1 2 2	
1.280E-01	1.780E+01	29.99	B403	1 2 2 2 2	
1.409E-01	1.960E+01	30.3	A400	2 1 2 2 2	
1.930E-01	2.685E+01	34.9	A400	2 1 2 2 2	
1.718E-01	2.390E+01	37.99	B403	1 2 2 2 2	
2.026E-01	2.818E+01	40	D006	1 2 0 1 1	
2.085E-01	2.900E+01	40	D059	1 2 1 1 1	
3.021E+00	4.203E+02	40.60	E032	1 2 1 2 2	
2.678E-01	3.726E+01	40.70	E032	1 2 1 2 2	
3.081E+00	4.286E+02	42.50	E032	1 2 1 2 2	
2.961E+00	4.120E+02	42.70	E032	1 2 1 2 2	
3.196E+00	4.447E+02	49.70	E032	1 2 1 2 2	
4.350E-01	6.052E+01	50	D069	1 2 0 0 2	
4.148E-01	5.770E+01	50	F300	1 0 0 0 2	

(continued)

678. C₆H₅NO₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.096E-01	4.306E+01	53.30	E032	1 2 1 2 2	
2.900E+00	4.034E+02	54.90	E032	1 2 1 2 2	
3.423E-01	4.762E+01	55.10	E032	1 2 1 2 2	
3.305E+00	4.598E+02	60.70	E032	1 2 1 2 2	
2.834E+00	3.942E+02	65.00	E032	1 2 1 2 2	
3.986E-01	5.545E+01	67.80	E032	1 2 1 2 2	
5.021E-01	6.985E+01	69.40	E032	1 2 1 2 2	
2.768E+00	3.850E+02	73.30	E032	1 2 1 2 2	
3.406E+00	4.739E+02	75.70	E032	1 2 1 2 2	
6.553E-01	9.116E+01	78.30	E032	1 2 1 2 2	
6.837E-01	9.510E+01	79.80	E032	1 2 1 2 2	
2.699E+00	3.754E+02	80.30	E032	1 2 1 2 2	
7.124E-01	9.910E+01	80.70	E032	1 2 1 2 2	
7.987E-01	1.111E+02	82.30	E032	1 2 1 2 2	
9.431E-01	1.312E+02	85.70	E032	1 2 1 2 2	
2.555E+00	3.554E+02	86.00	E032	1 2 1 2 2	
1.076E+00	1.497E+02	88.50	E032	1 2 1 2 2	
2.398E+00	3.336E+02	89.70	E032	1 2 1 2 2	
1.320E+00	1.837E+02	90.70	E032	1 2 1 2 2	
1.438E+00	2.000E+02	91.30	E032	1 2 1 2 2	
2.234E+00	3.107E+02	91.30	E032	1 2 1 2 2	
1.664E+00	2.315E+02	92.10	E032	1 2 1 2 2	
2.056E+00	2.861E+02	92.70	E032	1 2 1 2 2	
1.763E+00	2.453E+02	92.80	E032	1 2 1 2 2	
1.865E+00	2.595E+02	92.90	E032	1 2 1 2 2	
3.503E+00	4.873E+02	93.50	E032	1 2 1 2 2	
5.100E-02	7.095E+00	ns	B157	0 0 0 0 1	
1.148E-01	1.597E+01	ns	R427	0 0 0 0 0	

679. C₆H₅NO₃

m-Nitrophenol

3-Nitrophenol

RN: 554-84-7

MP (°C): 97

MW: 139.11

BP (°C): 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.412E-02	8.920E+00	0	D006	1 2 0 1 1	
5.176E-02	7.200E+00	9.99	B403	1 2 2 2 2	
8.524E-02	1.186E+01	12.5	D006	1 2 0 1 1	
1.243E-01	1.730E+01	15.90	E032	1 2 1 2 2	
7.764E-02	1.080E+01	19.99	B403	1 2 2 2 2	
8.300E-02	1.155E+01	20	H306	1 0 1 2 1	
1.368E-01	1.903E+01	20.20	E032	1 2 1 2 2	
1.458E-01	2.028E+01	23.40	E032	1 2 1 2 2	
9.575E-02	1.332E+01	25	D006	1 2 0 1 2	
9.740E-02	1.355E+01	25	K040	1 0 2 1 2	
9.225E-02	1.283E+01	25	R041	0 0 0 0 0	

(continued)

679. C₆H₅NO₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.685E-01	2.344E+01	29.50	E032	1 2 1 2 2	
1.200E-01	1.670E+01	29.99	B403	1 2 2 2 2	
1.366E-01	1.900E+01	34.99	B403	1 2 2 2 2	
1.944E-01	2.705E+01	35.80	E032	1 2 1 2 2	
2.113E-01	2.940E+01	40	F300	1 0 0 0 2	
2.148E-01	2.988E+01	40.90	E032	1 2 1 2 2	
3.196E+00	4.445E+02	47.10	E032	1 2 1 2 2	
3.046E+00	4.237E+02	49.60	E032	1 2 1 2 2	
3.240E+00	4.507E+02	49.70	E032	1 2 1 2 2	
3.313E+00	4.609E+02	56.50	E032	1 2 1 2 2	
2.979E+00	4.145E+02	58.70	E032	1 2 1 2 2	
2.911E-01	4.049E+01	58.80	E032	1 2 1 2 2	
3.475E-01	4.834E+01	62.70	E032	1 2 1 2 2	
3.387E+00	4.712E+02	62.80	E032	1 2 1 2 2	
2.914E+00	4.054E+02	71.50	E032	1 2 1 2 2	
3.484E+00	4.846E+02	75.10	E032	1 2 1 2 2	
4.703E-01	6.542E+01	77.10	E032	1 2 1 2 2	
2.828E+00	3.935E+02	80.60	E032	1 2 1 2 2	
6.326E-01	8.801E+01	85.30	E032	1 2 1 2 2	
3.549E+00	4.937E+02	85.80	E032	1 2 1 2 2	
2.705E+00	3.762E+02	89.40	E032	1 2 1 2 2	
3.569E+00	4.965E+02	89.80	E032	1 2 1 2 2	
2.649E+00	3.684E+02	92.20	E032	1 2 1 2 2	
9.501E-01	1.322E+02	93.60	E032	1 2 1 2 2	
2.581E+00	3.591E+02	94.20	E032	1 2 1 2 2	
2.475E+00	3.443E+02	95.60	E032	1 2 1 2 2	
1.210E+00	1.683E+02	96.20	E032	1 2 1 2 2	
2.396E+00	3.333E+02	96.60	E032	1 2 1 2 2	
1.440E+00	2.004E+02	97.50	E032	1 2 1 2 2	
2.286E+00	3.181E+02	97.70	E032	1 2 1 2 2	
1.604E+00	2.232E+02	98.10	E032	1 2 1 2 2	
2.341E+00	3.256E+02	98.10	E032	1 2 1 2 2	
1.763E+00	2.453E+02	98.40	E032	1 2 1 2 2	
2.049E+00	2.851E+02	98.50	E032	1 2 1 2 2	
1.965E+00	2.734E+02	98.60	E032	1 2 1 2 2	
3.008E+00	4.184E+02	98.70	F300	1 0 0 0 2	
9.772E-02	1.359E+01	ns	R427	0 0 0 0 0	

680. C₆H₅NO₄

Nitrohydroquinone

2-Nitroquinol

4-Hydroxy-2-nitrophenol

RN: 16090-33-8 MP (°C):

MW: 155.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.888E-02	1.068E+01	30.20	E032	1 2 1 2 2	
1.015E-01	1.575E+01	34.60	E032	1 2 1 2 2	

(continued)

680. C₆H₅NO₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.572E-01	2.439E+01	44.60	E032	1 2 1 2 2	
1.999E-01	3.101E+01	49.60	E032	1 2 1 2 2	
3.128E-01	4.853E+01	54.50	E032	1 2 1 2 2	
4.498E-01	6.977E+01	59.10	E032	1 2 1 2 2	
6.405E-01	9.934E+01	61.70	E032	1 2 1 2 2	
7.163E-01	1.111E+02	64.20	E032	1 2 1 2 2	
8.409E-01	1.304E+02	65.00	E032	1 2 1 2 2	
1.074E+00	1.667E+02	93.80	E032	1 2 1 2 2	

681. C₆H₅NO₄

4-Nitroresorcinol

4-Nitro-1,3-benzenediol

RN: 3163-07-3 MP (°C):
 MW: 155.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.354E-02	6.754E+00	18.30	E032	1 2 1 2 2	
5.244E-02	8.133E+00	24.70	E032	1 2 1 2 2	
6.510E-02	1.010E+01	30.80	E032	1 2 1 2 2	
7.959E-02	1.235E+01	36.90	E032	1 2 1 2 2	
1.034E-01	1.604E+01	43.50	E032	1 2 1 2 2	
1.462E-01	2.267E+01	47.50	E032	1 2 1 2 2	
1.817E-01	2.818E+01	49.10	E032	1 2 1 2 2	
2.168E-01	3.363E+01	50.70	E032	1 2 1 2 2	
2.497E-01	3.874E+01	51.20	E032	1 2 1 2 2	
2.776E-01	4.306E+01	52.30	E032	1 2 1 2 2	
3.286E-01	5.096E+01	53.90	E032	1 2 1 2 2	
4.487E-01	6.959E+01	57.80	E032	1 2 1 2 2	
5.951E-01	9.231E+01	62.70	E032	1 2 1 2 2	
8.468E-01	1.313E+02	68.40	E032	1 2 1 2 2	
1.075E+00	1.667E+02	71.90	E032	1 2 1 2 2	
1.209E+00	1.875E+02	72.90	E032	1 2 1 2 2	
1.325E+00	2.055E+02	73.30	E032	1 2 1 2 2	
1.487E+00	2.307E+02	73.40	E032	1 2 1 2 2	

682. C₆H₅NO₄

2-Nitroresorcinol

2-Nitro-1,3-benzenediol

RN: 601-89-8 MP (°C): 81
 MW: 155.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.435E-03	1.308E+00	28.40	E032	1 2 1 2 2	
1.306E-02	2.026E+00	36.70	E032	1 2 1 2 2	
2.319E-02	3.597E+00	47.60	E032	1 2 1 2 2	
3.635E-02	5.638E+00	54.90	E032	1 2 1 2 2	

(continued)

682. C₆H₅NO₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.276E-02	9.734E+00	67.20	E032	1 2 1 2 2	
8.399E-02	1.303E+01	74.40	E032	1 2 1 2 2	
1.208E-01	1.874E+01	82.90	E032	1 2 1 2 2	
1.529E-01	2.372E+01	92.30	E032	1 2 1 2 2	

683. C₆H₅NO₄

3-Nitrocatechol

3-Nitro-1,2-benzenediol

RN: 6665-98-1 MP (°C):
 MW: 155.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.377E-02	8.340E+00	14.40	E032	1 2 1 2 2	
6.573E-02	1.019E+01	20.90	E032	1 2 1 2 2	
9.590E-02	1.488E+01	29.50	E032	1 2 1 2 2	
1.277E-01	1.980E+01	35.10	E032	1 2 1 2 2	
1.474E-01	2.286E+01	37.90	E032	1 2 1 2 2	
1.738E-01	2.695E+01	41.00	E032	1 2 1 2 2	
2.372E-01	3.679E+01	45.80	E032	1 2 1 2 2	
2.646E-01	4.104E+01	47.60	E032	1 2 1 2 2	
3.216E-01	4.988E+01	54.50	E032	1 2 1 2 2	
3.615E-01	5.607E+01	61.30	E032	1 2 1 2 2	
4.548E-01	7.055E+01	75.90	E032	1 2 1 2 2	
5.743E-01	8.909E+01	86.80	E032	1 2 1 2 2	
8.164E-01	1.266E+02	96.80	E032	1 2 1 2 2	

684. C₆H₅NO₄

4-Nitrocatechol

4-Nitro-1,2-benzenediol

RN: 3316-09-4 MP (°C):
 MW: 155.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.211E+00	1.878E+02	24.60	E032	1 2 1 2 2	
1.423E+00	2.208E+02	37.70	E032	1 2 1 2 2	
1.488E+00	2.308E+02	41.30	E032	1 2 1 2 2	
1.664E+00	2.582E+02	51.90	E032	1 2 1 2 2	
1.829E+00	2.837E+02	58.50	E032	1 2 1 2 2	
2.004E+00	3.109E+02	66.50	E032	1 2 1 2 2	
2.049E+00	3.179E+02	67.80	E032	1 2 1 2 2	
2.149E+00	3.334E+02	71.20	E032	1 2 1 2 2	

685. C₆H₅NO₅S*p*-Nitrobenzenesulfonic acid

4-Nitrobenzenesulfonic acid

RN: 138-42-1 **MP (°C):**
MW: 203.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.343E+00	4.760E+02	100.5	T023	1 2 2 1 2	
2.412E+00	4.901E+02	105.0	T023	1 2 2 1 2	
2.461E+00	5.000E+02	110.0	T023	1 2 2 1 2	

686. C₆H₅NO₅S.2H₂O*p*-Nitrobenzenesulfonic acid (dihydrate)

RN: 15481-55-7 **MP (°C):**
MW: 239.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E+00	3.987E+02	36.6	T023	1 2 2 1 2	
1.720E+00	4.113E+02	56.6	T023	1 2 2 1 2	
1.771E+00	4.235E+02	75.5	T023	1 2 2 1 2	
1.822E+00	4.359E+02	90.2	T023	1 2 2 1 2	
1.939E+00	4.638E+02	106.8	T023	1 2 2 1 2	
1.920E+00	4.592E+02	110.2	T023	1 2 2 1 2	

687. C₆H₅NO₅S.4H₂O*p*-Nitrobenzenesulfonic acid (tetrahydrate)

RN: 15481-55-7 **MP (°C):**
MW: 275.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E+00	2.919E+02	-8.3	T023	1 2 2 1 2	
1.146E+00	3.153E+02	-1.0	T023	1 2 2 1 2	
1.273E+00	3.504E+02	10.8	T023	1 2 2 1 2	
1.318E+00	3.627E+02	16.0	T023	1 2 2 1 2	
1.409E+00	3.877E+02	26.3	T023	1 2 2 1 2	

688. C₆H₅N₂OS

Methyl acetylthiodiazole

Thiodiazolique methyle acetyle

RN: **MP (°C):**
MW: 153.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.528E-04	1.000E-01	37	D084	1 0 1 0 1	

689. C₆H₅N₃

Benzotriazole

1,2,3-Benzotriazole

Cobratec 99

1,2,3-triaza-1H-indene

Azimidobenzene

Benzene azimide

RN: 95-14-7 **MP (°C):** 98.5**MW:** 119.13 **BP (°C):** 350

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-01	1.977E+01	ns	R427	0 0 0 0 0	

690. C₆H₅N₃O₄

2,6-Dinitroaniline

2,6-Dinitrobenzenamine

RN: 606-22-4 **MP (°C):** 133**MW:** 183.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-04	7.994E-02	25	B335	1 2 0 0 1	

691. C₆H₅N₃O₄

2,4-Dinitroaniline

2,4-Dinitrobenzenamine

2,4-Dinitroaminobenzene

1-Amino-2,4-dinitrobenzene

RN: 97-02-9 **MP (°C):** 176**MW:** 183.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-04	7.812E-02	25	B335	1 2 0 0 1	

692. C₆H₅N₃O₅

Picramic acid

2-Amino-4,6-dinitro-phenol

RN: 96-91-3 **MP (°C):** 169**MW:** 199.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.031E-03	1.400E+00	22	F300	1 0 0 0 1	

693. C₆H₅N₅

7-Aminopteridine

7-Pteridinamine

RN: 769-66-4 **MP (°C):**
MW: 147.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.851E-03	7.138E-01	20	A083	1 2 0 0 0	
3.974E-02	5.848E+00	100	A083	1 2 0 0 0	

694. C₆H₅N₅

4-Aminopteridine

4-Pteridinamine

RN: 6973-01-9 **MP (°C):** 305
MW: 147.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.851E-03	7.138E-01	22.5	A085	1 2 0 0 0	

695. C₆H₅N₅

2-Aminopteridine

2-Pteridinamine

RN: 700-81-2 **MP (°C):**
MW: 147.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.031E-03	7.402E-01	22.5	A085	1 2 0 0 0	

696. C₆H₅N₅O

4-Amino-2-hydroxypteridine

4-Amino-2-oxopteridine

4-Aminopteridin-2-one

4-Amino-2-pteridone

RN: 22005-65-8 **MP (°C):** >350
MW: 163.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.378E-04	7.142E-02	20	A019	2 2 1 1 2	
5.104E-03	8.326E-01	100	A019	1 2 1 1 2	

697. C₆H₅N₅O

2-Amino-4-hydroxypteridine

2-Amino-4(1H)-pteridinone

2-Amino-4(3H)-pteridinone

2-Amino-4-pteridone

2-Amino-4-oxopteridine

2-Aminopterin-4-one

RN: 2236-60-4 **MP (°C):****MW:** 163.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.075E-04	1.754E-02	22.5	A085	1 2 0 0 0	

698. C₆H₅N₅O

7-Amino-6-hydroxypteridine

7-Amino-6-oxopteridine

7-Aminopterin-6-one

7-Amino-6-pteridone

RN: 1008-85-1 **MP (°C):****MW:** 163.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-03	2.000E-01	100	A082	1 2 0 0 0	

699. C₆H₅N₅O₂

Xanthopterin

2-Amino-4:6-dihydroxypteridine

RN: 119-44-8 **MP (°C):****MW:** 179.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.396E-04	2.500E-02	22.5	A085	1 2 0 0 0	

700. C₆H₅N₅O₃

Leucopterin

2-Amino-4:6:7-trihydroxypteridine

RN: 492-11-5 **MP (°C):****MW:** 195.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.833E-06	1.333E-03	22.5	A085	1 2 0 0 0	

701. C₆H₅N₅O₄S

3'-Nitrosoniridazole

2-Imidazolidinone, 1-nitroso-3-(5-nitro-2-thiazolyl)-

RN: 34968-90-6 MP (°C): 202-203

MW: 243.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.084E-04	7.500E-02	25	G051	1 0 1 1 0	

702. C₆H₆

Benzene

Benzol

Phenyl hydride

Cyclohexatriene

Benzolene

Phene

RN: 71-43-2 MP (°C): 5

MW: 78.11 BP (°C): 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.350E-02	1.836E+00	.20	M151	2 1 2 2 2	
2.347E-02	1.833E+00	.24	M183	1 2 1 1 2	
1.959E-02	1.530E+00	0	F300	1 0 0 0 2	
2.148E-02	1.678E+00	0	P003	2 2 2 2 2	
2.356E-02	1.840E+00	.80	A004	1 2 2 1 2	
2.351E-02	1.837E+00	4.50	B086	2 1 2 2 2	
1.881E-02	1.469E+00	4.62	U013	1 0 0 0 0	EFG
2.646E-02	2.067E+00	4.8	L007	2 1 1 2 2	
1.178E-02	9.200E-01	5	S119	0 0 0 0 1	
2.646E-02	2.067E+00	5.0	L007	2 1 1 1 2	
1.838E-02	1.436E+00	5.39	U010	1 0 0 1 1	EFG
2.310E-02	1.804E+00	6.20	M151	2 1 2 2 2	
2.306E-02	1.802E+00	6.24	M183	1 2 1 1 2	
2.364E-02	1.847E+00	6.30	B086	2 1 2 2 2	
2.313E-02	1.807E+00	7.10	B086	2 1 2 2 2	
2.313E-02	1.807E+00	9	B086	2 1 2 2 2	
2.292E-02	1.790E+00	9.40	A004	1 2 2 1 2	
2.080E-02	1.625E+00	10	B149	2 1 1 2 2	
2.110E-02	1.648E+00	10	J302	2 1 2 2 2	
2.240E-02	1.750E+00	10	M130	1 0 0 0 2	
2.300E-02	1.797E+00	11.00	M151	2 1 2 2 2	
2.300E-02	1.796E+00	11.04	M183	1 2 1 1 2	
2.262E-02	1.767E+00	11.80	B086	2 1 2 2 2	
2.262E-02	1.767E+00	12.10	B086	2 1 2 2 2	
2.270E-02	1.773E+00	14.00	M151	2 1 2 2 2	
2.263E-02	1.767E+00	14.04	M183	1 2 1 1 2	
1.838E-02	1.436E+00	14.20	U013	1 0 0 0 0	EFG
2.655E-02	2.074E+00	14.8	L007	2 1 1 2 2	

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702. C₆H₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.655E-02	2.074E+00	14.9	L007	2 1 1 1 2	
2.290E-02	1.789E+00	15	I333	1 2 1 1 2	
2.150E-02	1.679E+00	15	S006	1 0 0 0 2	
1.971E-02	1.540E+00	15	S203	1 1 2 1 2	
1.797E-02	1.403E+00	15.02	U010	1 0 0 1 1	EFG
2.287E-02	1.787E+00	15.10	B086	2 1 2 2 2	
2.112E-02	1.650E+00	16	D047	1 0 0 1 2	
2.266E-02	1.770E+00	16.80	A004	1 2 2 1 2	
2.260E-02	1.765E+00	16.90	M151	2 1 2 2 2	
2.253E-02	1.760E+00	16.94	M183	1 2 1 1 2	
2.191E-02	1.711E+00	17	F002	2 2 2 2 2	
2.287E-02	1.787E+00	17.90	B086	2 1 2 2 2	
2.260E-02	1.765E+00	18.60	M151	2 1 2 2 2	
2.259E-02	1.764E+00	18.64	M183	1 2 1 1 2	
2.664E-02	2.081E+00	19.8	L007	2 1 1 2 2	
2.664E-02	2.081E+00	19.9	L007	2 1 1 1 2	
2.220E-02	1.734E+00	20	B149	2 1 1 2 2	
2.180E-02	1.703E+00	20	C006	1 2 1 1 2	
1.023E-02	7.994E-01	20	C121	0 0 0 0 0	unit assumed, <i>sic</i>
2.428E-02	1.896E+00	20	D052	1 1 0 0 1	
1.600E-02	1.250E+00	20	E009	1 0 0 0 1	
1.680E-02	1.312E+00	20	E025	1 0 2 2 2	
2.189E-02	1.710E+00	20	F071	1 1 2 1 2	
2.317E-02	1.810E+00	20	F300	1 0 0 0 2	
1.023E-02	7.994E-01	20	I310	0 0 0 0 0	
2.310E-02	1.804E+00	20	I333	1 2 1 1 2	
2.042E-02	1.595E+00	20	K337	1 0 0 0 2	
2.280E-02	1.781E+00	20	M312	1 0 0 0 1	
1.366E-02	1.067E+00	20	M337	2 1 2 2 2	
2.650E-02	2.070E+00	20	P073	1 0 0 1 2	
1.751E-02	1.368E+00	20.0	H043	2 2 2 2 2	
2.249E-02	1.757E+00	20.10	B086	2 1 2 2 2	
2.224E-02	1.737E+00	21	C024	2 1 1 2 2	
2.202E-02	1.720E+00	22	F002	2 2 2 2 2	
2.320E-02	1.812E+00	22.5	I333	1 2 1 1 2	
2.304E-02	1.800E+00	24	A004	1 2 2 1 2	
2.667E-02	2.084E+00	24.8	L007	2 1 1 2 2	
2.227E-02	1.740E+00	25	A001	1 2 2 2 2	
1.917E-02	1.498E+00	25	A037	2 2 2 2 2	
2.292E-02	1.790E+00	25	B003	2 2 2 2 2	
2.045E-02	1.597E+00	25	B019	1 0 1 2 0	
2.279E-02	1.780E+00	25	B060	2 0 1 1 1	
2.292E-02	1.790E+00	25	B090	2 2 2 1 2	
2.292E-02	1.790E+00	25	B151	1 2 2 1 2	
2.330E-02	1.820E+00	25	B153	2 1 1 1 2	
2.240E-02	1.750E+00	25	B173	2 0 2 2 2	
2.300E-02	1.797E+00	25	G323	2 2 2 2 2	
2.300E-02	1.797E+00	25	H332	2 2 2 2 1	
2.330E-02	1.820E+00	25	I333	1 2 1 1 2	

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702. C₆H₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.310E-02	1.804E+00	25	J302	2 1 2 2 2	
2.390E-02	1.867E+00	25	K001	2 2 2 2 2	
8.961E-03	7.000E-01	25	K072	1 0 1 1 1	
1.300E-02	1.015E+00	25	K123	1 0 2 2 1	
2.170E-02	1.695E+00	25	K316	2 2 2 2 2	
2.259E-02	1.765E+00	25	L002	2 2 2 2 2	
2.313E-02	1.807E+00	25	L319	1 0 2 1 1	
2.166E-02	1.692E+00	25	L322	1 1 2 2 1	
1.770E+00	1.383E+02	25	M021	2 2 2 1 2	sic
2.279E-02	1.780E+00	25	M131	1 0 0 0 2	
2.278E-02	1.780E+00	25	M132	2 2 2 1 2	
2.310E-02	1.804E+00	25	M151	2 1 2 2 2	average of 2
2.293E-02	1.791E+00	25	M151	2 1 1 2 2	
2.290E-02	1.789E+00	25	M342	1 0 1 1 2	
1.917E-02	1.498E+00	25	O015	0 0 0 0 0	
2.247E-02	1.755E+00	25	P003	2 2 2 2 2	
2.227E-02	1.740E+00	25	P051	2 1 1 2 2	
2.607E-02	2.036E+00	25	S010	2 1 2 1 2	
2.377E-02	1.857E+00	25	S012	2 0 2 2 2	
2.061E-02	1.610E+00	25	S203	1 1 2 1 2	
2.070E-02	1.617E+00	25	S359	2 1 2 2 2	
2.778E-02	2.170E+00	25	W057	2 0 2 2 2	
2.290E-02	1.789E+00	25	W300	2 2 2 2 2	
2.300E-02	1.797E+00	25.0	H043	2 2 2 2 2	
2.667E-02	2.084E+00	25.0	L007	2 1 1 1 2	
2.227E-02	1.740E+00	25.00	P007	2 1 2 2 2	
2.290E-02	1.789E+00	25.04	M183	1 2 1 1 2	
1.838E-02	1.436E+00	25.35	U010	1 0 0 1 1	EFG
1.881E-02	1.469E+00	25.35	U013	1 0 0 0 0	EFG
2.325E-02	1.816E+00	25.84	M183	1 2 1 1 2	
2.213E-02	1.729E+00	26	F002	2 2 2 2 2	
2.229E-02	1.742E+00	29	F002	2 2 2 2 2	
2.351E-02	1.837E+00	29.99	C349	0 0 0 0 0	
2.368E-02	1.850E+00	30	F300	1 0 0 0 2	
2.364E-02	1.847E+00	30	G029	1 0 2 2 2	
2.350E-02	1.836E+00	30	I333	1 2 1 1 2	
2.343E-02	1.830E+00	31	A004	1 2 2 1 2	
2.285E-02	1.785E+00	32	F002	2 2 2 2 2	
1.970E-02	1.539E+00	34.53	U013	1 0 0 0 0	EFG
2.685E-02	2.098E+00	34.8	L007	2 1 1 2 2	
2.329E-02	1.819E+00	35	F002	2 2 2 2 2	
2.253E-02	1.760E+00	35	S203	1 1 2 1 2	
2.685E-02	2.098E+00	35.1	L007	2 1 1 1 2	
1.925E-02	1.504E+00	35.48	U010	1 0 0 1 1	EFG
2.458E-02	1.920E+00	38	A004	1 2 2 1 2	
2.573E-02	2.010E+00	39.99	C349	0 0 0 0 0	
2.592E-02	2.025E+00	40	B151	1 2 1 1 2	
2.434E-02	1.902E+00	41	F002	2 2 2 2 2	
2.440E-02	1.906E+00	42	F002	2 2 2 2 2	

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702. C₆H₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.467E-02	1.927E+00	44	F002	2 2 2 2 2	
2.016E-02	1.574E+00	44.30	U010	1 0 0 1 1	EFG
2.062E-02	1.611E+00	44.30	U013	1 0 0 0 0	EFG
2.599E-02	2.030E+00	44.70	A004	1 2 2 1 2	
2.368E-02	1.850E+00	45	S203	1 1 2 1 2	
2.938E-02	2.295E+00	45.7	L007	2 1 1 1 2	
2.938E-02	2.295E+00	45.8	L007	2 1 1 2 2	
2.534E-02	1.979E+00	46	F002	2 2 2 2 2	
2.827E-02	2.208E+00	49.99	C349	0 0 0 0 0	
2.810E-02	2.195E+00	50	G323	2 2 2 2 1	
2.650E-02	2.070E+00	51	F002	2 2 2 2 2	
2.740E-02	2.140E+00	51.50	A004	1 2 2 1 2	
2.159E-02	1.687E+00	53.64	U010	1 0 0 1 1	EFG
2.210E-02	1.726E+00	54.71	U013	1 0 0 0 0	EFG
5.095E-02	3.980E+00	55.3	P051	2 1 1 2 2	
5.095E-02	3.980E+00	55.30	P007	2 1 2 2 2	
2.788E-02	2.178E+00	56	F002	2 2 2 2 2	
3.162E-02	2.470E+00	57	B124	2 2 2 1 2	
3.776E-02	2.950E+00	57.70	B124	1 2 2 1 2	
2.996E-02	2.340E+00	58.80	A004	1 2 2 1 2	
3.131E-02	2.446E+00	59.99	C349	0 0 0 0 0	
2.938E-02	2.295E+00	60	B126	1 0 1 1 1	
3.101E-02	2.422E+00	60	B151	1 2 1 1 2	
2.943E-02	2.299E+00	61	F002	2 2 2 2 2	
3.004E-02	2.347E+00	63	F002	2 2 2 2 2	
3.290E-02	2.570E+00	65.40	A004	1 2 2 1 2	
2.479E-02	1.936E+00	65.82	U013	1 0 0 0 0	EFG
3.597E-02	2.810E+00	69.20	B124	1 2 2 1 2	
3.587E-02	2.802E+00	69.30	B124	1 0 2 2 2	
3.463E-02	2.705E+00	69.99	C349	0 0 0 0 0	
8.280E-02	6.468E+00	74.7	P051	2 1 1 2 2	
8.280E-02	6.468E+00	74.70	P007	2 1 2 2 2	
3.872E-02	3.024E+00	79.99	C349	0 0 0 0 0	
4.429E-02	3.460E+00	89.99	C349	0 0 0 0 0	
2.560E-02	2.000E+00	100	J023	1 1 2 2 0	
5.256E-02	4.106E+00	99.99	C349	0 0 0 0 0	
7.681E-02	6.000E+00	150	J023	1 1 2 2 0	
2.688E-01	2.100E+01	200	J023	1 1 2 2 1	
9.345E-01	7.300E+01	250	J023	1 1 2 2 1	
1.357E+00	1.060E+02	285	J023	1 1 2 2 2	
1.869E+00	1.460E+02	300	J023	1 1 2 2 2	
2.200E-02	1.719E+00	ns	B059	0 0 1 1 2	
4.000E-03	3.125E-01	ns	D348	0 0 0 0 0	
2.279E-02	1.780E+00	ns	H123	0 0 0 0 0	
3.020E-01	2.359E+01	ns	H307	0 0 0 0 0	
4.500E-02	3.515E+00	ns	H333	0 1 0 1 0	EFG
2.330E-02	1.820E+00	ns	I332	0 0 0 0 2	
2.292E-02	1.790E+00	ns	K304	0 0 0 0 2	
1.933E-02	1.510E+00	ns	M010	0 0 0 0 2	

(continued)

702. C₆H₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E-02	1.769E+00	ns	M175	0 0 2 1 2	
2.279E-02	1.780E+00	ns	M344	0 0 0 0 2	

703. C₆H₆BrNO₂S

4-Bromobenzenesulfonamide

(4-Bromophenyl)sulfonamide

p-Bromobenzenesulfonamide

4-Aminosulfonyl-1-bromobenzene

RN: 701-34-8 **MP (°C):****MW:** 236.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	9.916E-01	15	K024	1 2 1 1 2	

704. C₆H₆BrNO₃S*p*-Bromoaniline-*o*-sulfonic acid

2-Amino-5-bromophenylsulfonic acid

RN: 1576-59-6 **MP (°C):****MW:** 252.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.107E-02	2.790E+00	8.35	P038	1 0 1 0 2	anhydride
1.424E-02	3.590E+00	16.75	P038	1 0 1 0 2	anhydride
1.769E-02	4.460E+00	25.0	P038	1 0 1 0 2	anhydride
2.578E-02	6.500E+00	40.0	P038	1 0 1 0 2	anhydride
3.828E-02	9.650E+00	55.0	P038	1 0 1 0 2	anhydride
5.454E-02	1.375E+01	70.0	P038	1 0 1 0 2	anhydride
8.013E-02	2.020E+01	85.0	P038	1 0 1 0 2	anhydride
8.846E-03	2.230E+00	.0	P038	1 0 1 0 2	anhydride

705. C₆H₆BrNO₃S*p*-Bromoaniline-*m*-sulfonic acid

5-Amino-2-bromobenzenesulfonic acid

RN: 150454-14-1 **MP (°C):****MW:** 252.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.511E-02	8.850E+00	9.8	P038	1 2 2 2 2	anhydrous rhombic
2.559E-02	6.450E+00	12.55	P038	1 2 2 2 2	anhydrous monoclinic
4.284E-02	1.080E+01	20.0	P038	1 2 2 2 2	anhydrous rhombic
3.419E-02	8.620E+00	25.0	P038	1 2 2 2 2	anhydrous monoclinic
4.740E-02	1.195E+01	25.0	P038	1 2 2 2 2	anhydrous rhombic
5.177E-02	1.305E+01	29.6	P038	1 2 2 2 2	anhydrous rhombic
5.732E-02	1.445E+01	34.7	P038	1 2 2 2 2	anhydrous rhombic
4.820E-02	1.215E+01	40.0	P038	1 2 2 2 2	anhydrous monoclinic

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705. C₆H₆BrNO₃S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.387E-02	1.610E+01	40.1	P038	1 2 2 2 2	anhydrous rhombic
6.922E-02	1.745E+01	44.5	P038	1 2 2 2 2	anhydrous rhombic
7.577E-02	1.910E+01	49.7	P038	1 2 2 2 2	anhydrous rhombic
8.330E-02	2.100E+01	54.8	P038	1 2 2 2 2	anhydrous rhombic
7.101E-02	1.790E+01	56.3	P038	1 2 2 2 2	anhydrous monoclinic
9.600E-02	2.420E+01	62.3	P038	1 2 2 2 2	anhydrous rhombic
9.679E-02	2.440E+01	70.0	P038	1 2 2 2 2	anhydrous monoclinic
1.115E-01	2.810E+01	70.4	P038	1 2 2 2 2	anhydrous rhombic
1.329E-01	3.350E+01	85.0	P038	1 2 2 2 2	anhydrous monoclinic
1.452E-01	3.660E+01	85.0	P038	1 2 2 2 2	anhydrous rhombic
2.880E-02	7.260E+00	.0	P038	1 2 2 2 2	anhydrous rhombic
1.884E-02	4.750E+00	.0	P038	1 2 2 2 2	anhydrous monoclinic

706. C₆H₆BrNO₃S.H₂O*p*-Bromoaniline-*o*-sulfonic acid (monohydrate)

2-Amino-5-bromophenylsulfonic acid (monohydrate)

RN: 1576-59-6 MP (°C):

MW: 270.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	3.520E+00	8.35	P038	1 0 1 0 2	monohydrate
1.751E-02	4.730E+00	16.8	P038	1 0 1 0 2	monohydrate
2.244E-02	6.060E+00	25.0	P038	1 0 1 0 2	monohydrate
9.589E-03	2.590E+00	.0	P038	1 0 1 0 2	monohydrate

707. C₆H₆ClN*p*-Chloroaniline

4-Chloroaniline

RN: 106-47-8 MP (°C): 72.5

MW: 127.57 BP (°C): 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.157E-02	2.752E+00	20	H118	1 1 1 1 2	
2.157E-02	2.752E+00	20	H301	0 0 0 0 0	
3.057E-02	3.900E+00	22.5	G301	0 0 0 0 0	

708. C₆H₆ClN*o*-Chloroaniline

2-Chloroaniline

RN: 95-51-2 MP (°C): -1

MW: 127.57 BP (°C): 208.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-02	3.765E+00	20	C113	1 0 2 1 2	

709. C₆H₆ClN*m*-Chloroaniline

3-Chloroaniline

RN: 108-42-9

MP (°C): -10

MW: 127.57

BP (°C): 230.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.266E-02	5.442E+00	20	C113	1 0 2 1 2	

710. C₆H₆ClNO₂S*m*-Chlorobenzenesulfonamide

MON 5783

RN: 17260-71-8

MP (°C):

MW: 191.64

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-03	6.707E-01	15	K024	1 2 1 1 2	

711. C₆H₆ClNO₂S*o*-Chlorobenzenesulfonamide

2-Chlorobenzenesulfonamide

RN: 6961-82-6

MP (°C):

MW: 191.64

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-03	4.983E-01	15	K024	1 2 1 1 2	

712. C₆H₆ClNO₂S*4*-Chlorobenzenesulfonamide*p*-Chlorobenzenesulfonamide

RN: 98-64-6

MP (°C):

MW: 191.64

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.322E+00	15	K024	1 2 1 1 2	

713. C₆H₆ClNO₃S*p*-Chloroaniline-*m*-sulfonic acid

1-Amino-4-chlorobenzene-3-sulfonic acid

4-Chloro-3-sulfoaniline

3-Amino-6-chlorobenzenesulfonic acid

RN: 88-43-7

MP (°C):

MW: 207.64

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.447E-02	1.131E+01	0	P038	1 0 1 1 2	anhydride

714. C₆H₆ClNO₃S.H₂O*p*-Chloroaniline-*o*-sulfonic acid (monohydrate)

1-Amino-4-chloro-2-benzenesulfonic acid (monohydrate)

RN: 133-74-4 **MP (°C):****MW:** 225.65 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.387E-02	3.130E+00	0	P038	1 2 2 1 2	monohydrate

715. C₆H₆ClNO₃S.H₂O*p*-Chloroaniline-*m*-sulfonic acid (monohydrate)

1-Amino-4-chlorobenzene-3-sulfonic acid (monohydrate)

RN: 88-43-7 **MP (°C):****MW:** 225.65 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.141E-02	1.160E+01	0	P038	1 0 1 1 2	metastable monohydrate

716. C₆H₆Cl₆ β -1,2,3,4,5,6-Hexachlorocyclohexane β -Benzene hexachloride β -BHC β -Hexachlorocyclohexane**RN:** 319-85-7 **MP (°C):** 312**MW:** 290.83 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.719E-05	5.000E-03	20	C099	1 2 0 0 0	
8.252E-07	2.400E-04	25	W025	1 0 2 2 2	
5.501E-07	1.600E-04	28	K120	1 2 2 2 1	average of 2
1.719E-06	5.000E-04	ns	M061	0 0 0 0 0	

717. C₆H₆Cl₆ δ -1,2,3,4,5,6-Hexachlorocyclohexane δ -Benzene hexachloride**RN:** 608-73-1 **MP (°C):****MW:** 290.83 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
1.080E-04	3.140E-02	25	W025	1 0 2 2 2	
4.009E-05	1.166E-02	28	K120	1 2 2 2 2	average of 4

718. C₆H₆Cl₆

Lindane

γ-BHC

Benzene hexachloride

RN: 58-89-9 **MP (°C):** 112.5
MW: 290.83 **BP (°C):** 0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.393E-06	2.150E-03	15	B083	2 2 1 2 2	
7.393E-06	2.150E-03	15	B162	1 0 0 0 2	
2.816E-05	8.190E-03	19	I018	1 0 0 0 2	
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
2.709E-05	7.880E-03	22	K137	1 1 2 1 0	
2.706E-05	7.870E-03	24	C313	0 0 0 0 0	
5.845E-05	1.700E-02	24	H116	2 1 0 0 2	
2.338E-05	6.800E-03	25	B083	2 2 1 2 2	
2.338E-05	6.800E-03	25	B162	1 0 0 0 2	
2.586E-05	7.520E-03	25	M060	2 2 1 2 2	
2.510E-05	7.300E-03	25	M130	1 0 0 0 1	
2.682E-05	7.800E-03	25	W025	1 0 2 2 2	
4.126E-05	1.200E-02	27	B161	2 1 2 2 0	EFG
2.235E-05	6.500E-03	28	K120	1 2 2 2 2	average of 4 particle size 5 μm
3.920E-05	1.140E-02	35	B083	2 2 1 2 2	
7.221E-05	2.100E-02	35	B161	2 1 2 2 0	EFG
3.920E-05	1.140E-02	35	B162	1 0 0 0 2	
5.226E-05	1.520E-02	45	B083	2 2 1 2 2	particle size 5 μm
9.284E-05	2.700E-02	45	B161	2 1 2 2 0	
1.135E-04	3.300E-02	50	B161	2 1 2 2 0	EFG
1.547E-04	4.500E-02	60	B161	2 1 2 2 0	EFG
2.400E-05	6.980E-03	ns	C318	0 0 0 0 0	
~3.44E-05	~1.00E-02	ns	I308	0 0 0 0 0	
5.158E-07	1.500E-04	ns	K138	0 0 0 0 2	sic
3.438E-06	1.000E-03	ns	M061	0 0 0 0 0	
2.407E-05	7.000E-03	ns	M110	0 0 0 0 0	EFG
2.510E-05	7.300E-03	ns	V414	0 0 0 0 0	
3.438E-05	1.000E-02	rt	M161	0 0 0 0 1	

719. C₆H₆Cl₆

α-1,2,3,4,5,6-Hexachlorocyclohexane

α-Benzene hexachloride

α-HCH

α-BHC

α-Hexachlorocyclohexane

RN: 319-84-6 **MP (°C):** 158
MW: 290.83 **BP (°C):** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.438E-05	1.000E-02	20	C099	1 2 0 0 1	
6.877E-06	2.000E-03	25	W025	1 0 2 2 2	
5.570E-06	1.620E-03	28	K120	1 2 2 2 2	average of 4
3.438E-06	1.000E-03	ns	M061	0 0 0 0 0	

720. C₆H₆FN₃O₃

1-Methylcarbamoyl-5-fluorouracil

5-Fluoro-3,4-dihydro-*N*-methyl-2,4-dioxo-pyrimidinecarboxamide

1-Methylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

RN: 56563-18-9 **MP (°C):** 225–228**MW:** 187.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.313E-03	6.200E-01	22	B321	0 0 0 0 0	pH 4.0
3.313E-03	6.200E-01	22	B388	0 0 0 0 0	

721. C₆H₆INO₃S

2-Iodoaniline-4-sulphonic acid

Benzenesulfonic acid, 4-amino-2-iodo-

RN: 67877-88-7 **MP (°C):****MW:** 299.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.781E-02	2.028E+01	25	B107	1 2 1 1 2	

722. C₆H₆INO₃S

3-Iodoaniline-4-sulphonic acid

Benzenesulfonic acid, 4-amino-3-iodo-

RN: 25210-30-4 **MP (°C):****MW:** 299.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.474E-03	1.936E+00	25	B107	1 2 1 1 2	

723. C₆H₆INO₃S

4-Iodoaniline-2-sulphonic acid

Benzenesulfonic acid, 2-amino-4-iodo-

RN: 171664-62-3 **MP (°C):****MW:** 299.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.697E-02	5.074E+00	25	B107	1 2 1 1 1	

724. C₆H₆INO₃S

4-Iodoaniline-3-sulphonic acid

Benzenesulfonic acid, 3-amino-4-iodo-

RN: **MP (°C):****MW:** 299.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.486E-02	1.342E+01	25	B107	1 2 1 1 2	

725. C₆H₆INO₃S

5-Iodoaniline-2-sulphonic acid

Benzenesulfonic acid, 2-amino-5-iodo-

RN: MP (°C):

MW: 299.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.671E-03	2.593E+00	25	B107	1 2 1 1 1	

726. C₆H₆INO₃S

6-Iodoaniline-3-sulphonic acid

Benzenesulfonic acid, 3-amino-6-iodo-

RN: MP (°C):

MW: 299.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.597E-02	4.777E+00	25	B107	1 2 1 1 1	

727. C₆H₆INO₃S

5-Iodoaniline-3-sulphonic acid

Benzenesulfonic acid, 3-amino-5-iodo-

RN: MP (°C):

MW: 299.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.323E-02	1.293E+01	25	B107	1 2 1 1 2	

728. C₆H₆N₂O

Nicotiamide

Niacinamide

Nicotinamide

RN: 98-92-0 MP (°C): 131

MW: 122.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.094E+00	5.000E+02	20	D041	1 0 0 0 2	
8.188E+00	1.000E+03	20	M054	1 0 0 0 2	
2.900E-03	3.542E-01	25	A350	0 0 0 0 0	
8.188E+00	1.000E+03	25	D315	0 0 0 0 0	
8.188E-01	1.000E+02	ns	K444	0 0 0 0 0	

729. C₆H₆N₂O₂

3-Nitroaniline

1-Amino-3-nitrobenzene

3-Nitrobenzenamine

m-Nitroaminobenzene*m*-Nitroaniline

3-Nitro-anilin

RN: 99-09-2**MP (°C):** 114**MW:** 138.13**BP (°C):** 306

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.710E-03	1.203E+00	20	B179	0 0 0 0 0	
5.370E-03	7.418E-01	25	B335	1 2 0 0 1	
6.516E-03	9.000E-01	25	F300	1 0 0 0 2	
3.020E-03	4.171E-01	25	L016	1 0 0 0 2	unit assumed
6.582E-03	9.092E-01	25.0	C026	0 0 0 0 0	
1.290E-02	1.782E+00	40.1	C026	0 0 0 0 0	

730. C₆H₆N₂O₂

Urocanic acid

Urocaninsaeure

RN: 104-98-3**MP (°C):** 225**MW:** 138.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E-02	1.500E+00	17.40	F300	1 0 0 0 1	
4.318E-02	5.964E+00	37	D041	1 0 0 0 0	
5.575E-02	7.700E+00	50	F300	1 0 0 0 1	
4.098E-01	5.660E+01	100	D041	1 0 0 0 0	

731. C₆H₆N₂O₂*p*-Nitroaniline

4-Amino-nitrobenzene

Benzenamine

4-Nitroaniline

p-Aminonitrobenzene

4-Nitrobenzenamine

RN: 100-01-6**MP (°C):** 146**MW:** 138.13**BP (°C):** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.754E-03	7.948E-01	20	B179	0 0 0 0 0	
2.823E-03	3.900E-01	20	H300	1 2 2 2 1	<i>sic</i>
2.815E-03	3.888E-01	20	T301	1 2 2 2 2	
3.020E-03	4.171E-01	25	B335	1 2 0 0 1	
4.344E-03	6.000E-01	25	F300	1 0 0 0 2	<i>sic</i>
5.370E-03	7.418E-01	25	L016	1 0 0 0 2	unit assumed
4.110E-03	5.677E-01	25.0	C026	0 0 0 0 0	
5.267E-03	7.275E-01	30	G029	1 0 2 2 2	
8.367E-03	1.156E+00	40.1	C026	0 0 0 0 0	

732. C₆H₆N₂O₂

2-Nitroaniline

o-Nitroaniline

1-Amino-2-nitrobenzene

2-Nitro-aniline

RN: 88-74-4**MP (°C):** 71.5**MW:** 138.13**BP (°C):** 284

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.467E-03	8.932E-01	20	T301	1 2 2 2 2	
8.764E-03	1.211E+00	25.0	C026	0 0 0 0 0	
1.750E-02	2.417E+00	40.1	C026	0 0 0 0 0	
6.134E-03	8.473E-01	50	T301	1 2 2 2 2	average of 4
6.799E-03	9.391E-01	80	T301	1 2 2 2 2	average of 4

733. C₆H₆N₂O₃

5,5-Ethylenebarbituric acid

Spirocyclopropane-1',5-barbituric acid

5,7-Diazaspiro[2.5]octane-4,6,8-trione

Cyclopropane-spirobarbiturate

RN: 6947-77-9 **MP (°C):****MW:** 154.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.004E+00	25	P350	0 0 0 0 0	intrinsic

734. C₆H₆N₂O₄

1-Methylorotic acid

4-Pyrimidinecarboxylic acid, 1,2,3,6-tetrahydro-1-methyl-2,6-dioxo-

RN: 705-36-2 **MP (°C):****MW:** 170.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.042E+01	20	N019	0 0 0 0 0	

735. C₆H₆N₂O₄S*m*-Nitrobenzenesulfonamide

3-Nitrobenzenesulfonamide

RN: 121-52-8 **MP (°C):****MW:** 202.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	4.448E-01	15	K024	1 2 1 1 2	

736. C₆H₆N₂O₄S

4-Nitrobenzenesulfonamide

p-Nitrobenzenesulfonamide**RN:** 6325-93-5 **MP (°C):****MW:** 202.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	6.066E-01	15	K024	1 2 1 1 2	

737. C₆H₆N₂O₄S

2-Nitrobenzenesulfonamide

o-Nitrobenzenesulfonamide**RN:** 5455-59-4 **MP (°C):****MW:** 202.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	3.235E-01	15	K024	1 2 1 1 2	

738. C₆H₆N₄

8-Methylpurine

1H-Purine, 8-methyl-

RN: 934-33-8 **MP (°C):****MW:** 134.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.924E-01	5.263E+01	20	A022	1 0 0 0 0	

739. C₆H₆N₄O

8-Hydroxymethylpurine

Purine-8-methanol

RN: 6642-26-8 **MP (°C):****MW:** 150.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.014E-02	4.525E+00	20	A022	1 2 0 0 0	
4.440E-01	6.667E+01	100	A082	1 2 0 0 0	

740. C₆H₆N₄O₃

9-Methyluric acid

1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-9-methyl-

*N*9-Methyluric acid**RN:** 55441-71-9 **MP (°C):****MW:** 182.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.999E-03	5.461E-01	ns	B115	0 0 1 1 0	

741. C₆H₆N₄O₃

1-Methyluric acid

 α -Methyluric acid

RN: 708-79-2

MP (°C): 400

MW: 182.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-02	2.101E+00	ns	B115	0 0 1 1 0	ζ form
8.701E-03	1.585E+00	ns	B115	0 0 1 1 0	γ form
2.731E-02	4.975E+00	ns	B115	0 0 1 1 0	
2.754E-02	5.017E+00	ns	R427	0 0 0 0 0	

742. C₆H₆N₄O₃S

Niridazole

Nirodazole

RN: 61-57-4

MP (°C): 261

MW: 214.20

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.068E-04	1.300E-01	25	A081	1 0 1 1 0	EFG
1.634E-04	3.500E-02	25	G051	1 0 1 1 0	pH 2

743. C₆H₆N₄O₄

5-Nitro-2-furaldehyde semicarbazone

Nitrofurazone

RN: 59-87-0

MP (°C): 236

MW: 198.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.225E-04	1.630E-01	ns	B404	0 2 1 1 0	
1.201E-03	2.380E-01	ns	I310	0 0 0 0 0	
8.128E-04	1.611E-01	ns	R427	0 0 0 0 0	

744. C₆H₆N₆

2,4-Diaminopteridine

2:4-Diaminopteridine

RN: 1127-93-1

MP (°C):

MW: 162.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.055E-03	3.332E-01	20	A019	2 2 1 1 2	
4.708E-02	7.634E+00	100	A019	1 2 1 1 1	

745. C₆H₆N₆

4,6-Diaminopteridine

4:6-Diaminopteridine

RN: 19167-60-3 **MP (°C):****MW:** 162.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.569E-04	4.166E-02	20	A020	1 2 0 1 1	
6.554E-03	1.063E+00	100	A020	1 2 0 0 0	

746. C₆H₆N₆

4,7-Diaminopteridine

4:7-Diaminopteridine

RN: 771-41-5 **MP (°C):****MW:** 162.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-03	2.000E-01	20	A020	1 2 0 0 1	
2.049E-02	3.322E+00	100	A020	1 2 0 0 0	

747. C₆H₆N₆

4-Hydrazinopteridine

4(1H)-Pteridinone, hydrazone

RN: 77632-11-2 **MP (°C):****MW:** 162.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-02	2.217E+00	20	A083	1 2 0 0 0	
8.686E-02	1.408E+01	100	A083	1 2 0 0 0	

748. C₆H₆O

Phenol

Carbolic acid

Hydroxybenzene

RN: 108-95-2 **MP (°C):** 40.85**MW:** 94.11 **BP (°C):** 182

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.164E-01	6.743E+01	0	A056	1 0 1 1 2	
7.136E-01	6.716E+01	0	B031	1 2 2 2 1	
7.164E-01	6.743E+01	0	L059	1 0 1 1 2	
6.858E-01	6.455E+01	8.60	C058	2 0 2 1 1	
7.321E-01	6.890E+01	10	A056	1 0 1 1 2	
7.321E-01	6.890E+01	10	L059	1 0 1 1 2	
8.080E-01	7.604E+01	15.1	A400	2 1 2 2 2	

(continued)

748. C₆H₆O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.672E-01	6.279E+01	16	D041	1 0 0 0 1	
7.779E-01	7.322E+01	20	B031	1 2 2 2 1	
8.710E-01	8.197E+01	20	B179	0 0 0 0 0	
4.866E+00	4.580E+02	20	C052	1 2 1 1 2	sic
8.235E-01	7.750E+01	20	F300	1 0 0 0 2	
8.198E-01	7.715E+01	20	H003	1 2 2 1 2	
1.600E+00	1.506E+02	20	H306	1 0 1 2 1	
8.500E-01	8.000E+01	20	K119	1 0 0 0 2	
7.130E-01	6.710E+01	20	K301	2 2 1 1 2	
6.175E-01	5.811E+01	20	R087	0 0 0 0 0	0.15M NaCl
9.490E-01	8.931E+01	22.70	M135	1 2 1 1 2	
1.000E+00	9.411E+01	25	A021	1 2 1 1 0	
8.930E-01	8.405E+01	25	A400	2 1 2 2 2	
9.882E-01	9.300E+01	25	B060	2 0 1 1 1	
9.400E-01	8.847E+01	25	B316	0 0 0 0 0	
9.000E-01	8.470E+01	25	F044	1 0 0 0 1	
8.468E-01	7.970E+01	25	H003	1 2 2 1 2	
8.245E-01	7.759E+01	25	H028	2 0 2 0 2	
1.527E-01	1.437E+01	25	K129	2 1 2 2 2	
8.854E-01	8.333E+01	25	L022	1 0 0 0 0	
9.000E-01	8.470E+01	25	L088	1 0 0 0 1	
7.413E-01	6.977E+01	25	M041	1 1 0 0 1	
9.300E-01	8.753E+01	25	P031	0 0 0 0 0	
7.688E-01	7.236E+01	25	R041	0 0 0 0 0	
9.900E-01	9.317E+01	26.90	M135	1 2 1 1 2	
8.970E-01	8.442E+01	30	H003	1 2 2 1 2	
8.297E-01	7.809E+01	30	V009	1 0 0 0 1	
1.048E+00	9.863E+01	32.20	M135	1 2 1 1 2	
9.598E-01	9.033E+01	34	B063	1 2 2 1 2	
9.892E-01	9.310E+01	35	A400	2 1 2 2 2	
9.580E-01	9.016E+01	35	H003	1 2 2 1 2	
1.107E+00	1.042E+02	36.00	M135	1 2 1 1 2	
9.130E-01	8.592E+01	40	B031	1 2 2 2 1	
1.158E+00	1.090E+02	43.70	M135	1 2 1 1 2	
1.369E+00	1.288E+02	47.70	M135	1 2 1 1 2	
1.172E+00	1.103E+02	48.00	C058	2 0 2 1 2	
1.138E+00	1.071E+02	50	M041	1 1 0 0 2	
1.476E+00	1.389E+02	50.50	M135	1 2 1 1 2	
1.183E+00	1.113E+02	51.90	B063	1 2 2 1 2	
1.592E+00	1.498E+02	53.50	M135	1 2 1 1 2	
1.725E+00	1.623E+02	55.80	M135	1 2 1 1 2	
1.388E+00	1.306E+02	55.90	B063	1 2 2 1 2	
1.375E+00	1.295E+02	57.30	H003	1 2 2 1 2	
1.856E+00	1.747E+02	57.80	M135	1 2 1 1 2	
1.590E+00	1.497E+02	60	B031	1 2 2 2 2	
2.163E+00	2.036E+02	60.90	M135	1 2 1 1 2	
1.612E+00	1.518E+02	61.70	B063	1 2 2 1 2	
1.723E+00	1.621E+02	62.74	H003	1 2 2 1 2	
1.771E+00	1.667E+02	63.20	B063	1 2 2 1 2	

(continued)

748. C₆H₆O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E+00	1.985E+02	65.40	B063	1 2 2 1 2	
3.064E+00	2.884E+02	65.50	B063	1 2 2 1 2	
2.567E+00	2.416E+02	65.55	B063	1 2 2 1 2	
2.767E+00	2.604E+02	65.60	B063	1 2 2 1 2	
2.388E+00	2.247E+02	65.79	H003	1 2 2 1 2	average of 2
2.590E+00	2.437E+02	65.84	H003	1 2 2 1 2	
2.624E+00	2.469E+02	65.86	H003	1 2 2 1 2	
2.536E+00	2.387E+02	65.90	H003	1 2 2 1 2	
2.818E+00	2.652E+02	66.0	H068	2 0 0 0 2	
2.397E+00	2.256E+02	66.01	H003	1 2 2 1 2	
1.734E+00	1.632E+02	66.30	C058	2 0 2 1 2	
8.243E-01	7.758E+01	ns	A406	0 0 0 0 1	
8.594E-01	8.088E+01	ns	N330	2 2 2 1 2	
8.710E-01	8.197E+01	ns	R427	0 0 0 0 0	
8.043E-01	7.570E+01	rt	N051	0 0 2 1 2	average of 3

749. C₆H₆O₂

Hydroquinone

Hydrochinon

Hydroquinol

RN: 123-31-9

MP (°C): 173.5

MW: 110.11

BP (°C): 286

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.493E-01	3.846E+01	0	M043	1 0 0 0 1	
4.653E-01	5.123E+01	10	M043	1 0 0 0 1	
4.904E-01	5.400E+01	15	F300	1 0 0 0 1	
5.077E-01	5.590E+01	17.70	L065	1 0 0 0 2	0.01N HCl
5.087E-01	5.601E+01	17.90	L065	1 0 0 0 2	0.01N HCl
5.101E-01	5.617E+01	17.95	L065	1 0 0 0 2	0.01N HCl
5.103E-01	5.619E+01	18	L064	2 2 2 1 2	0.01N HCl
6.100E-01	6.716E+01	20	M043	1 0 0 0 1	
6.357E-01	7.000E+01	22.5	G301	0 0 0 0 0	
6.180E-01	6.805E+01	23.75	L064	2 2 2 1 2	0.01N HCl
6.450E-01	7.102E+01	25	G033	1 0 1 1 2	
7.283E-01	8.020E+01	25	K033	1 0 0 1 2	
6.660E-01	7.334E+01	25	K040	1 0 2 1 2	
7.955E-01	8.759E+01	30	M043	1 0 0 0 1	
1.045E+00	1.150E+02	40	M043	1 0 0 0 1	
2.354E+00	2.593E+02	60	M043	1 0 0 0 1	
5.694E+00	6.270E+02	75.3	W038	2 2 2 1 2	
4.251E+00	4.681E+02	80	M043	1 0 0 0 1	
7.528E+00	8.289E+02	81.9	W038	2 2 2 1 2	
6.034E+00	6.644E+02	100	M043	1 0 0 0 2	
1.961E+01	2.159E+03	114.6	W038	2 2 2 1 2	
2.180E+01	2.400E+03	120.3	W038	2 2 2 1 2	
2.728E+01	3.004E+03	131.7	W038	2 2 2 1 2	

(continued)

749. C₆H₆O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.942E+01	3.239E+03	136.0	W038	2 2 2 1 2	
3.353E+01	3.692E+03	141.8	W038	2 2 2 1 2	
3.621E+01	3.987E+03	147.2	W038	2 2 2 1 2	
6.026E-01	6.635E+01	ns	R427	0 0 0 0 0	
6.084E-01	6.699E+01	rt	D021	0 0 1 1 2	

750. C₆H₆O₂

Pyrocatechol
Brenzkatechin
Catechol

RN: 120-80-9 **MP (°C):** 105
MW: 110.11 **BP (°C):** 245.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.824E+00	3.110E+02	20	F300	1 0 0 0 2	
2.823E+00	3.108E+02	20	M043	1 0 0 0 2	
4.190E+00	4.614E+02	25	K040	1 0 2 1 2	
5.743E+00	6.324E+02	40	M043	1 0 0 0 2	
1.278E+01	1.408E+03	41.2	W038	2 2 2 1 2	
2.061E+01	2.270E+03	56.7	W038	2 2 2 1 2	
2.068E+01	2.278E+03	57.1	W038	2 2 2 1 2	
7.308E+00	8.047E+02	60	M043	1 0 0 0 2	
2.617E+01	2.882E+03	66.2	W038	2 2 2 1 2	
8.337E+00	9.180E+02	80	M043	1 0 0 0 2	
8.974E+00	9.882E+02	100	M043	1 0 0 0 2	
5.556E+01	6.117E+03	104.5	W038	2 2 2 1 2	
2.823E+00	3.108E+02	rt	D021	0 0 1 1 2	

751. C₆H₆O₂

Resorcinol
Resorcin

RN: 108-46-3 **MP (°C):** 110.0
MW: 110.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.404E+00	3.748E+02	0	M022	1 0 0 0 2	
3.617E+00	3.983E+02	0	M043	1 0 0 0 2	
2.784E+00	3.066E+02	3.70	L090	1 0 0 1 2	
4.173E+00	4.595E+02	10	M043	1 0 0 0 1	
5.413E+00	5.960E+02	12.50	F300	1 0 0 0 2	
3.186E+00	3.508E+02	14.20	L090	1 0 0 1 2	
3.359E+00	3.699E+02	19.50	L090	1 0 0 1 2	
4.576E+00	5.038E+02	20	M022	1 0 0 0 2	
5.009E+00	5.516E+02	20	M043	1 0 0 0 2	
6.515E+00	7.174E+02	25	K040	1 0 2 1 2	

(continued)

751. C₆H₆O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.330E+00	6.970E+02	30	F300	1 0 0 0 2	
5.718E+00	6.296E+02	30	M043	1 0 0 0 2	
3.679E+00	4.051E+02	32.50	L090	1 0 0 1 2	
1.464E+01	1.612E+03	33.61	W038	2 2 2 1 2	
5.641E+00	6.211E+02	40	M022	1 0 0 0 2	
6.287E+00	6.923E+02	40	M043	1 0 0 0 2	
1.843E+01	2.030E+03	44.5	W038	2 2 2 1 2	
2.042E+01	2.249E+03	49.3	W038	2 2 2 1 2	
2.100E+01	2.312E+03	50.4	W038	2 2 2 1 2	
6.465E+00	7.119E+02	60	M022	1 0 0 0 2	
7.228E+00	7.959E+02	60	M043	1 0 0 0 2	
2.701E+01	2.974E+03	64.4	W038	2 2 2 1 2	
2.997E+01	3.300E+03	70.7	W038	2 2 2 1 2	
7.106E+00	7.825E+02	80	M022	1 0 0 0 2	
7.844E+00	8.638E+02	80	M043	1 0 0 0 2	
3.516E+01	3.871E+03	80.5	W038	2 2 2 1 2	
4.008E+01	4.414E+03	88.5	W038	2 2 2 1 2	
7.592E+00	8.360E+02	100	M022	1 0 0 0 2	
8.299E+00	9.138E+02	100	M043	1 0 0 0 2	
5.556E+01	6.117E+03	109.4	W038	2 2 2 1 2	
4.608E+00	5.074E+02	rt	D021	0 0 1 1 2	

752. C₆H₆O₃

Maltol

3-Hydroxy-2-methyl-4-pyrone

Hydroxymethylpyrone

Palatone

RN: 118-71-8 MP (°C): 161.5

MW: 126.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.643E-02	1.090E+01	15	F300	1 0 0 0 2	

753. C₆H₆O₃

Methyl furoate

5-Methyl-brenzschleimsaeure

5-Methylfuroic acid

RN: 611-13-2 MP (°C):

MW: 126.11 BP (°C): 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-01	1.860E+01	20	F300	1 0 0 0 2	

754. C₆H₆O₃

Phloroglucinol

1,3,5-Benzenetriol

1,3,5-Trihydroxybenzene

1,3,5-THB

RN: 108-73-6

MP (°C): 218.0

MW: 126.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.405E-02	1.060E+01	20	F300	1 0 0 0 2	
8.860E-02	1.117E+01	rt	D021	0 0 1 1 2	

755. C₆H₆O₃

Pyrogallol

1,2,3-Trihydroxybenzene

1,2,3-Benzenetriol

Brown AP

Fourrine 85

RN: 87-66-1

MP (°C): 131

MW: 126.11

BP (°C): 309

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.379E+00	3.000E+02	13	F300	1 0 0 0 0	average
3.013E+00	3.800E+02	25	F300	1 0 0 0 1	
4.020E+00	5.070E+02	25	K040	1 0 2 1 2	

756. C₆H₆O₃S

Benzenesulfonic acid

Benzolsulfosaeure

RN: 98-11-3

MP (°C): 43

MW: 158.18

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.088E+00	4.885E+02	31.4	T023	1 2 2 1 2	
3.109E+00	4.917E+02	42.6	T023	1 2 2 1 2	
3.136E+00	4.960E+02	56.0	T023	1 2 2 1 2	
3.154E+00	4.989E+02	61.3	T023	1 2 2 1 2	

757. C₆H₆O₃S.H₂O

Benzenesulfonic acid (monohydrate)

RN: 98-11-3

MP (°C):

MW: 176.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E+00	4.478E+02	21.3	T023	1 2 2 1 2	
2.568E+00	4.525E+02	31.0	T023	1 2 2 1 2	
2.770E+00	4.881E+02	32.6	T023	1 2 2 1 2	

(continued)

757. C₆H₆O₃S.H₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.598E+00	4.577E+02	39.5	T023	1 2 2 1 2	
2.751E+00	4.846E+02	39.8	T023	1 2 2 1 2	
2.722E+00	4.796E+02	49.0	T023	1 2 2 1 2	
2.641E+00	4.654E+02	49.0	T023	1 2 2 1 2	
2.682E+00	4.726E+02	52.4	T023	1 2 2 1 2	

758. C₆H₆O₃S.2.5H₂O

Benzenesulfonic acid (2.5 hydrate)

RN: 98-11-3 MP (°C):
MW: 203.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.107E+00	4.281E+02	-4.0	T023	1 2 2 1 2	
2.122E+00	4.312E+02	-3.3	T023	1 2 2 1 2	
2.150E+00	4.370E+02	-2.3	T023	1 2 2 1 2	
2.131E+00	4.331E+02	-2.5	T023	1 2 2 1 2	

759. C₆H₆O₃S.2H₂O

Benzenesulfonic acid (dihydrate)

RN: 98-11-3 MP (°C):
MW: 194.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.250E+00	4.370E+02	2.2	T023	1 2 2 1 2	
2.265E+00	4.399E+02	7.5	T023	1 2 2 1 2	
2.289E+00	4.446E+02	13.7	T023	1 2 2 1 2	
2.297E+00	4.460E+02	15.1	T023	1 2 2 1 2	

760. C₆H₆O₃S.3H₂O

Benzenesulfonic acid (trihydrate)

RN: 98-11-3 MP (°C):
MW: 212.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E+00	3.586E+02	-40.8	T023	1 2 2 1 2	
1.766E+00	3.748E+02	-29.0	T023	1 2 2 1 2	
1.842E+00	3.909E+02	-18.5	T023	1 2 2 1 2	
1.922E+00	4.078E+02	-10.0	T023	1 2 2 1 2	
1.975E+00	4.191E+02	-5.9	T023	1 2 2 1 2	
2.011E+00	4.267E+02	-4.7	T023	1 2 2 1 2	

761. C₆H₆O₄

Muconic acid

Muconsaeure

RN: 505-70-4

MP (°C):

MW: 142.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.407E-03	2.000E-01	20	F300	1 0 0 0 2	

762. C₆H₇F₃N₄OS

Thiazafluron

Urea, N,N'-dimethyl-N-[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]-

RN: 25366-23-8 MP (°C): 136.5

MW: 240.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.724E-03	2.096E+00	20	E048	1 2 1 1 2	
8.742E-03	2.100E+00	20	M161	1 0 0 0 1	

763. C₆H₇N

Aniline

Aminobenzene

C.I. Oxidation base 1

Aminophen

Kyanol

RN: 62-53-3 MP (°C): -6.3

MW: 93.13 BP (°C): 184

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.531E-01	3.288E+01	8.60	C058	2 0 2 1 1	
3.877E-01	3.611E+01	13.8	K119	1 0 0 0 2	
3.747E-01	3.490E+01	18	F300	1 0 0 0 2	
3.818E-01	3.556E+01	18.15	P057	0 0 0 0 0	
3.612E-01	3.364E+01	22	H072	1 0 1 1 2	
3.930E-01	3.660E+01	22.5	G301	0 0 0 0 0	
3.931E-01	3.661E+01	25	B019	1 0 1 2 0	
3.931E-01	3.661E+01	25	B092	2 1 1 1 2	
4.000E-01	3.725E+01	25	F044	1 0 0 0 1	
3.791E-01	3.531E+01	25	G323	2 2 2 2 2	
3.800E-01	3.539E+01	25	H028	2 0 2 0 2	
3.791E-01	3.531E+01	25	H078	1 2 1 0 2	
3.650E-01	3.399E+01	25	M116	2 1 1 1 2	
3.731E-01	3.475E+01	25.40	C058	2 0 2 1 1	
3.930E-01	3.660E+01	26.70	L095	2 2 1 1 2	
4.229E-01	3.939E+01	48.00	C058	2 0 2 1 1	
4.328E-01	4.031E+01	50	G323	2 2 2 2 2	
5.016E-01	4.671E+01	60	B092	2 1 1 1 2	
5.016E-01	4.671E+01	66.30	C058	2 0 2 1 1	
7.025E-01	6.542E+01	96.70	C058	2 0 2 1 1	
3.801E-01	3.540E+01	ns	A406	0 0 0 0 1	

764. C₆H₇NO*m*-Aminophenol

3-Aminophenol

RN: 591-27-5

MP (°C): 125

MW: 109.13

BP (°C): 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.797E-01	1.961E+01	10	M043	1 0 0 0 1	
2.291E-01	2.500E+01	20	F300	1 0 0 0 1	
2.409E-01	2.629E+01	20	M043	1 0 0 0 1	
3.355E-01	3.661E+01	30	M043	1 0 0 0 1	
3.261E-01	3.559E+01	32.6	S120	1 2 1 1 2	
4.859E-01	5.303E+01	40	M043	1 0 0 0 1	
6.788E-01	7.407E+01	47.9	S120	1 2 1 1 2	
8.850E-01	9.658E+01	53.0	S120	1 2 1 1 2	
1.590E+00	1.736E+02	60	M043	1 0 0 0 1	
1.406E+00	1.535E+02	60.4	S120	1 2 1 1 2	
2.148E+00	2.344E+02	66.4	S120	1 2 1 1 2	
2.627E+00	2.866E+02	68.9	S120	1 2 1 1 2	
2.927E+00	3.194E+02	70.2	S120	1 2 1 1 2	
3.161E+00	3.450E+02	71.5	S120	1 2 1 1 2	
3.410E+00	3.721E+02	73.2	S120	1 2 1 1 2	
3.737E+00	4.078E+02	77.2	S120	1 2 1 1 2	
6.752E+00	7.368E+02	80	M043	1 0 0 0 2	
4.098E+00	4.472E+02	85.2	S120	1 2 1 1 2	
4.311E+00	4.705E+02	96.0	S120	1 2 1 1 2	
8.291E+00	9.048E+02	100	M043	1 0 0 0 2	

765. C₆H₇NO*o*-Aminophenol

2-Amino-phenol

RN: 95-55-6

MP (°C): 172

MW: 109.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.558E-01	1.700E+01	0	F300	1 0 0 0 1	
1.532E-01	1.672E+01	0	M043	1 0 0 0 1	
1.709E-01	1.865E+01	10	M043	1 0 0 0 1	
1.797E-01	1.961E+01	20	M043	1 0 0 0 1	
1.973E-01	2.153E+01	30	M043	1 0 0 0 1	
2.148E-01	2.344E+01	40	M043	1 0 0 0 1	
2.409E-01	2.629E+01	60	M043	1 0 0 0 1	
2.669E-01	2.913E+01	80	M043	1 0 0 0 1	
2.686E-01	2.931E+01	80.8	S120	1 2 1 1 1	
3.558E-01	3.883E+01	88.0	S120	1 2 1 1 1	
5.995E-01	6.542E+01	100	M043	1 0 0 0 1	

766. C₆H₇NO*p*-Aminophenol

4-Aminophenol

RN: 123-30-8**MP (°C):** 190**MW:** 109.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.008E-01	1.100E+01	0	F300	1 0 0 0 1	
9.970E-02	1.088E+01	0	M043	1 0 0 0 1	
1.176E-01	1.283E+01	10	M043	1 0 0 0 1	
1.443E-01	1.575E+01	20	M043	1 0 0 0 1	
1.709E-01	1.865E+01	30	M043	1 0 0 0 1	
2.060E-01	2.248E+01	40	M043	1 0 0 0 1	
2.678E-01	2.922E+01	59.0	S120	1 2 1 1 1	
3.184E-01	3.475E+01	60	M043	1 0 0 0 1	
5.544E-01	6.050E+01	77.0	S120	1 2 1 1 1	
6.709E-01	7.322E+01	80	M043	1 0 0 0 1	
8.399E-01	9.165E+01	86.7	S120	1 2 1 1 1	
1.497E+00	1.634E+02	96.6	S120	1 2 1 1 1	
2.475E+00	2.701E+02	100	M043	1 0 0 0 1	

767. C₆H₇NO

Phenylhydroxylamine

Phenylhydroxylamin

RN: 100-65-2**MP (°C):** 82**MW:** 109.13**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.833E-01	2.000E+01	5	F300	1 0 0 0 0	
8.247E-01	9.000E+01	100	F300	1 0 0 0 0	

768. C₆H₇NO₂S

Benzenesulfonamide

Benzolsulfosaeure-amid

RN: 98-10-2**MP (°C):** 151**MW:** 157.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-02	2.515E+00	15	K024	1 2 1 1 2	
2.736E-02	4.300E+00	16	F300	1 0 0 0 1	

769. C₆H₇NO₃S

Orthanilic acid

Orthanilsaeure

RN: 88-21-1

MP (°C): 325

MW: 173.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.525E-02	1.130E+01	8.25	P038	1 1 2 1 2	monohydrate
7.535E-02	1.305E+01	12.3	P038	1 1 2 1 2	monohydrate
8.459E-02	1.465E+01	15.55	P038	1 1 2 1 2	anhydrate
8.776E-02	1.520E+01	16.75	P038	1 1 2 1 2	anhydrate
1.114E-01	1.930E+01	25	P038	1 1 2 1 2	anhydrate
1.738E-01	3.010E+01	41.3	P038	1 1 2 1 2	anhydrate
2.477E-01	4.290E+01	55.0	P038	1 1 2 1 2	anhydrate
3.672E-01	6.360E+01	70.0	P038	1 1 2 1 2	anhydrate
5.185E-01	8.980E+01	85.0	P038	1 1 2 1 2	anhydrate
4.585E-02	7.940E+00	.0	P038	1 1 2 1 2	monohydrate

770. C₆H₇NO₃S

Sulfanilic acid

4-Aminobenzenesulfonic acid

Sulfanilsaeure

RN: 121-57-3

MP (°C): 122

MW: 173.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.672E-02	6.359E+00	0	D077	1 0 0 1 1	
2.587E-02	4.480E+00	0	M043	1 0 0 0 1	
4.810E-02	8.330E+00	10	D077	1 0 0 1 1	
4.850E-02	8.400E+00	10	F300	1 0 0 0 1	
4.583E-02	7.937E+00	10	M043	1 0 0 0 1	
6.169E-02	1.068E+01	20	D077	1 0 0 1 2	
5.774E-02	1.000E+01	20	F300	1 0 0 0 1	
6.395E-02	1.108E+01	20	M043	1 0 0 0 2	
8.477E-02	1.468E+01	30	D077	1 0 0 1 2	
1.115E-01	1.932E+01	40	D077	1 0 0 1 2	
1.109E-01	1.920E+01	40	F300	1 0 0 0 2	
1.149E-01	1.990E+01	40	M043	1 0 0 0 2	
1.414E-01	2.449E+01	50	D077	1 0 0 1 2	
1.736E-01	3.007E+01	60	D077	1 0 0 1 2	
1.687E-01	2.922E+01	60	M043	1 0 0 0 2	
2.159E-01	3.740E+01	69.9	P038	1 0 2 1 2	anhydrate
2.103E-01	3.642E+01	70	D077	1 0 0 1 2	
2.492E-01	4.315E+01	80	D077	1 0 0 1 2	
2.492E-01	4.315E+01	80	M043	1 0 0 0 2	
2.737E-01	4.740E+01	85.0	P038	1 0 2 1 2	anhydrate
3.031E-01	5.249E+01	90	D077	1 0 0 1 2	
3.610E-01	6.253E+01	100	D077	1 0 0 1 2	
3.851E-01	6.670E+01	100	F300	1 0 0 0 2	
3.610E-01	6.253E+01	100	M043	1 0 0 0 2	
6.075E-02	1.052E+01	ns	K076	0 0 0 0 2	

771. C₆H₇NO₃S

Metanilic acid

3-Aminobenzenesulfonic acid

m-Sulfanilic acid**RN:** 121-47-1**MP (°C):** >300**MW:** 173.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.901E-02	1.022E+01	7.75	P038	1 2 2 1 2	anhydrate
7.622E-02	1.320E+01	16.75	P038	1 2 2 1 2	anhydrate
9.440E-02	1.635E+01	24.95	P038	1 2 2 1 2	anhydrate
1.383E-01	2.395E+01	40.0	P038	1 2 2 1 2	anhydrate
1.975E-01	3.420E+01	55.0	P038	1 2 2 1 2	anhydrate
2.714E-01	4.700E+01	70.0	P038	1 2 2 1 2	anhydrate
4.561E-02	7.900E+00	.0	P038	1 2 2 1 2	anhydrate

772. C₆H₇NO₃S.1.5H₂O

Metanilic acid (sesquihydrate)

3-Aminobenzenesulfonic acid (sesquihydrate)

RN: 121-47-1**MP (°C):****MW:** 200.21**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.041E-02	1.610E+01	8.35	P038	1 2 2 1 2	
1.119E-01	2.240E+01	15.55	P038	1 2 2 1 2	
1.184E-01	2.370E+01	16.8	P038	1 2 2 1 2	
3.247E-01	6.500E+01	85.0	P038	1 2 2 1 2	
5.344E-02	1.070E+01	.0	P038	1 2 2 1 2	

773. C₆H₇NO₄S

2-Aminophenol-4-sulfonic acid

2-Amino-phenol-sulfosaeure-(4)

RN: 98-37-3**MP (°C):** >300**MW:** 189.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.286E-02	1.000E+01	14	F300	1 0 0 0 0	

774. C₆H₇NO₄S

4-Aminophenol-2-sulfonic acid

4-Amino-phenol-sulfosaeure-(2)

RN: 2835-04-3**MP (°C):****MW:** 189.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	7.000E-01	14	F300	1 0 0 0 0	

775. C₆H₇N₃O

Isoniazid

Isonicotinic acid hydrazide

laniazid

RN: 54-85-3**MP (°C):** 171**MW:** 137.14**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.813E-01	1.071E+02	20	I307	0 0 0 0 0	
8.955E-01	1.228E+02	25	B187	0 0 0 0 0	
1.458E+00	2.000E+02	37	I307	0 0 0 0 0	
1.505E+00	2.063E+02	40	B187	0 0 0 0 0	
9.115E-01	1.250E+02	ns	K444	0 0 0 0 0	

776. C₆H₇N₃O₃

Orotic acid methylamide

Orotamide, *N*-methyl-**RN:** 1009-04-7**MP (°C):** 284–286**MW:** 169.14**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.420E-01	5.785E+01	−4	N018	0 0 0 0 0	
6.840E-01	1.157E+02	16	N018	0 0 0 0 0	
8.340E-01	1.411E+02	25	N018	0 0 0 0 0	

777. C₆H₇N₇

2,4,7-Triaminopteridine

2:4:7-Triaminopteridine

RN: 14439-13-5**MP (°C):****MW:** 177.17**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.254E-03	2.222E-01	20	A020	1 2 0 0 1	
2.808E-02	4.975E+00	100	A020	1 2 0 0 0	

778. C₆H₇N₇

4,6,7-Triaminopteridine

4:6:7-Triaminopteridine

RN: 19167-62-5**MP (°C):****MW:** 177.17**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.515E-04	7.999E-02	20	A020	1 2 0 1 1	
1.252E-02	2.217E+00	100	A020	1 2 0 0 1	

779. C₆H₇O₂P

Phenylphosphinic acid

Phenyl-phosphinigsaeure

RN: 1779-48-2 **MP (°C):** 84
MW: 142.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.757E-01	6.760E+01	14	F300	1 0 0 0 2	
9.460E+00	1.344E+03	24.63	W422	0 0 0 0 0	
1.109E+01	1.576E+03	27.09	W422	0 0 0 0 0	
1.294E+01	1.839E+03	29.24	W422	0 0 0 0 0	
1.593E+01	2.264E+03	32.06	W422	0 0 0 0 0	
2.177E+01	3.093E+03	36.77	W422	0 0 0 0 0	
3.047E+01	4.330E+03	39.68	W422	0 0 0 0 0	
4.843E+00	6.881E+02	100	F300	1 0 0 0 2	

780. C₆H₇O₃P

Phenylphosphonic acid

Phenylphosphonsaeure

RN: 1571-33-1 **MP (°C):** 164.5
MW: 158.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E+00	1.900E+02	15	F300	1 0 0 0 2	
1.202E+00	1.901E+02	ns	R427	0 0 0 0 0	

781. C₆H₇O₃As

Benzeneearsonic acid

Phenylarsonsaeure

RN: 98-05-5 **MP (°C):** 160
MW: 202.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.564E-01	3.160E+01	28	F300	1 0 0 0 2	
9.899E-01	2.000E+02	84	F300	1 0 0 0 1	

782. C₆H₈

1,4-Cyclohexadiene

1,4-Dihydrobenzene

RN: 628-41-1 **MP (°C):** -49.2
MW: 80.13 **BP (°C):** 81

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-02	8.512E-01	4.8	L007	2 2 1 2 2	
1.062E-02	8.512E-01	5.1	L007	2 1 1 1 2	
1.195E-02	9.576E-01	14.8	L007	2 2 1 2 2	

(continued)

782. C₆H₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.195E-02	9.576E-01	15.2	L007	2 1 1 1 2	
8.002E-03	6.412E-01	20	M337	2 1 2 2 2	
1.167E-02	9.353E-01	24.8	L007	2 2 1 2 2	
8.736E-03	7.000E-01	25	M001	2 1 2 2 2	
1.167E-02	9.353E-01	25.1	L007	2 1 1 1 2	
1.201E-02	9.625E-01	34.8	L007	2 2 1 2 2	
1.201E-02	9.625E-01	35.2	L007	2 1 1 1 2	
1.259E-02	1.009E+00	44.8	L007	2 2 1 2 2	
1.259E-02	1.009E+00	45.2	L007	2 1 1 1 2	

783. C₆H₈ClN₇O

Amiloride

RN: 2609-46-3

MP (°C):

MW: 229.63

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.531E-04	1.500E-01	22.5	B422	0 0 0 0 0	
2.870E+00	6.590E+02	25	B443	0 0 0 0 0	

784. C₆H₈N₂

2,5-Dimethylpyrazine

2,5-Dimethyl-pyrazin

RN: 123-32-0

MP (°C): 63

MW: 108.14

BP (°C): 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		25	D425	0 0 0 0 0	

785. C₆H₈N₂

m-Phenylenediamine

m-Phenyldiamin

RN: 108-45-2

MP (°C): 63

MW: 108.14

BP (°C): 283

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.409E-01	8.012E+01	.3	S115	1 2 1 1 2	α form
2.928E-01	3.166E+01	.3	S115	1 2 1 1 2	β form
1.038E+00	1.122E+02	4.6	S115	1 2 1 1 2	α form
1.354E+00	1.465E+02	9.3	S115	1 2 1 1 2	α form
1.618E+00	1.750E+02	11.7	S115	1 2 1 1 2	α form
7.806E-01	8.442E+01	14.3	S115	1 2 1 1 2	β form
2.285E+00	2.472E+02	16.1	S115	1 2 1 1 2	α form
2.671E+00	2.889E+02	17.3	S115	1 2 1 1 2	α form
1.038E+00	1.122E+02	18.3	S115	1 2 1 1 2	β form
3.075E+00	3.326E+02	18.7	S115	1 2 1 1 2	α form
3.339E+00	3.611E+02	19.9	S115	1 2 1 1 2	α form

(continued)

785. C₆H₈N₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.537E+00	3.825E+02	20.8	S115	1 2 1 1 2	α form
1.354E+00	1.465E+02	22.0	S115	1 2 1 1 2	β form
3.796E+00	4.105E+02	22.7	S115	1 2 1 1 2	α form
1.480E+00	1.600E+02	23.1	S115	1 2 1 1 2	β form
1.618E+00	1.750E+02	24.1	S115	1 2 1 1 2	β form
1.918E+00	2.074E+02	25.1	S115	1 2 1 1 2	β form
3.979E+00	4.303E+02	26.0	S115	1 2 1 1 2	α form
2.285E+00	2.472E+02	26.3	S115	1 2 1 1 2	β form
2.671E+00	2.889E+02	27.1	S115	1 2 1 1 2	β form
2.815E+00	3.044E+02	27.1	S115	1 2 1 1 2	β form
3.075E+00	3.326E+02	27.9	S115	1 2 1 1 2	β form
4.085E+00	4.418E+02	28.7	S115	1 2 1 1 2	α form
3.339E+00	3.611E+02	29.0	S115	1 2 1 1 2	β form
3.537E+00	3.825E+02	29.1	S115	1 2 1 1 2	β form
3.796E+00	4.105E+02	30.2	S115	1 2 1 1 2	β form
3.979E+00	4.303E+02	31.5	S115	1 2 1 1 2	β form
4.217E+00	4.560E+02	32.6	S115	1 2 1 1 2	α form
4.085E+00	4.418E+02	32.8	S115	1 2 1 1 2	β form
4.217E+00	4.560E+02	34.4	S115	1 2 1 1 2	β form
4.439E+00	4.800E+02	43.5	S115	1 2 1 1 2	α form
4.549E+00	4.919E+02	53.6	S115	1 2 1 1 2	α form
4.586E+00	4.960E+02	57.6	S115	1 2 1 1 2	α form
4.623E+00	5.000E+02	62.8	S115	1 2 1 1 2	α form

786. C₆H₈N₂*o*-Phenylenediamine*o*-Phenylenediamin

RN: 95-54-5

MP (°C): 102–103

MW: 108.14

BP (°C): 257

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.876E-01	3.110E+01	20	T301	1 2 2 2 2	
3.763E-01	4.070E+01	35	F300	1 0 0 0 2	
3.599E-01	3.892E+01	35.1	S115	1 2 1 1 2	
5.110E-01	5.527E+01	45.8	S115	1 2 1 1 2	
9.804E-01	1.060E+02	56.3	S115	1 2 1 1 2	
1.458E+00	1.577E+02	61.3	S115	1 2 1 1 2	
1.755E+00	1.898E+02	62.8	S115	1 2 1 1 2	
2.218E+00	2.398E+02	64.2	S115	1 2 1 1 2	
2.948E+00	3.188E+02	66.1	S115	1 2 1 1 2	
3.558E+00	3.847E+02	67.7	S115	1 2 1 1 2	
3.955E+00	4.277E+02	71.3	S115	1 2 1 1 2	
4.338E+00	4.691E+02	80.8	S115	1 2 1 1 2	
4.476E+00	4.841E+02	88.1	S115	1 2 1 1 2	
4.533E+00	4.902E+02	91.7	S115	1 2 1 1 2	
4.570E+00	4.942E+02	95.5	S115	1 2 1 1 2	

787. C₆H₈N₂*p*-Phenylenediamine

1,4-Phenylenediamine

RN: 106-50-3 **MP (°C):** 141
MW: 108.14 **BP (°C):** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.880E-02	1.068E+01	3.6	S115	1 2 1 1 2	
3.299E-01	3.568E+01	23.7	S115	1 2 1 1 2	
4.180E-01	4.520E+01	25	F300	1 0 0 0 2	
8.292E-01	8.967E+01	37.8	S115	1 2 1 1 2	
1.460E+00	1.579E+02	49.9	S115	1 2 1 1 2	
1.978E+00	2.140E+02	59.2	S115	1 2 1 1 2	
2.368E+00	2.561E+02	64.6	S115	1 2 1 1 2	
2.724E+00	2.945E+02	69.2	S115	1 2 1 1 2	
3.155E+00	3.412E+02	75.5	S115	1 2 1 1 2	
3.432E+00	3.711E+02	80.3	S115	1 2 1 1 2	
3.809E+00	4.119E+02	88.5	S115	1 2 1 1 2	
4.055E+00	4.385E+02	95.9	S115	1 2 1 1 2	
1.500E-05	1.622E-03	98.59	M180	0 0 2 2 0	EFG
2.500E-05	2.704E-03	111.46	M180	0 0 2 2 0	EFG
4.000E-05	4.326E-03	117.47	M180	0 0 2 2 0	EFG
4.500E-05	4.866E-03	122.10	M180	0 0 2 2 0	EFG
5.000E-05	5.407E-03	126.84	M180	0 0 2 2 0	EFG
7.000E-05	7.570E-03	133.34	M180	0 0 2 2 0	EFG

788. C₆H₈N₂OS

5,6-Dimethyl-2-thiouracil

4(1H)-Pyrimidinone, 2,3-dihydro-5,6-dimethyl-2-thioxo-

5,6-Dimethylthiouracil

RN: 28456-54-4 **MP (°C):**
MW: 156.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.790E-03	1.373E+00	25	G016	1 2 1 2 2	intrinsic

789. C₆H₈N₂O₂*N,N*-1,3-Dimethyluracil

1,3-Dimethyl-2,4-pyrimidinedione

N1,N3-Dimethyluracil*N,N'*-Dimethyluracil

1,3-Dimethyluracil

RN: 874-14-6 **MP (°C):**
MW: 140.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.568E+00	5.000E+02	ns	B177	0 0 0 0 2	

790. C₆H₈N₂O₂S*o*-Aminobenzenesulfonamide

Orthanilamide

RN: 3306-62-5

MP (°C):

MW: 172.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-02	6.458E+00	23	K034	2 2 2 2 1	
3.865E-02	6.655E+00	24	K034	2 2 2 2 1	
4.323E-02	7.444E+00	26	K034	2 2 2 2 1	
4.723E-02	8.133E+00	28	K034	2 2 2 2 1	
5.237E-02	9.018E+00	30.5	K034	2 2 2 2 1	
5.806E-02	9.999E+00	33	K034	2 2 2 2 2	
6.034E-02	1.039E+01	34	K034	2 2 2 2 2	
6.375E-02	1.098E+01	35.5	K034	2 2 2 2 2	
6.886E-02	1.186E+01	37	K034	2 2 2 2 2	
6.829E-02	1.176E+01	37	K034	2 2 2 2 2	
8.356E-02	1.439E+01	42	K034	2 2 2 2 2	
9.707E-02	1.672E+01	46	K034	2 2 2 2 2	
1.139E-01	1.961E+01	50	K034	2 2 2 2 2	

791. C₆H₈N₂O₂S*m*-Aminobenzenesulfonamide

Metanilamide

m-Amidobenzenesulfonamide

RN: 98-18-0

MP (°C):

MW: 172.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.545E-02	1.127E+01	23	K034	2 2 2 2 2	
6.942E-02	1.196E+01	24	K034	2 2 2 2 2	
7.678E-02	1.322E+01	26	K034	2 2 2 2 2	
8.469E-02	1.458E+01	28	K034	2 2 2 2 2	
1.077E-01	1.855E+01	33	K034	2 2 2 2 2	
1.244E-01	2.143E+01	35.5	K034	2 2 2 2 2	
1.339E-01	2.306E+01	37	K034	2 2 2 2 2	
1.461E-01	2.515E+01	39	K034	2 2 2 2 2	
1.697E-01	2.922E+01	42	K034	2 2 2 2 2	
2.072E-01	3.568E+01	46	K034	2 2 2 2 2	
2.543E-01	4.379E+01	50	K034	2 2 2 2 2	

792. C₆H₈N₂O₂S

Benzenesulfamide

Sulfanilamide

Sulfanilsaeure-amid

p-Aminobenzenesulphonamide**RN:** 63-74-1**MP (°C):** 165**MW:** 172.21**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	1	A047	1 0 0 0 0	
1.057E-02	1.820E+00	4.40	B147	1 2 1 1 2	
1.458E-02	2.510E+00	10.20	B147	1 2 1 1 2	
1.957E-02	3.370E+00	15	B147	1 2 1 1 2	
2.323E-02	4.000E+00	15	F300	1 0 0 0 0	
2.660E-02	4.581E+00	15	K024	1 2 1 1 2	
2.241E-02	3.860E+00	15	S147	1 2 2 2 2	
2.889E-02	4.975E+00	16	A047	1 0 0 0 0	
2.439E-02	4.200E+00	16	H114	1 0 0 0 2	
2.700E-02	4.650E+00	20	B147	1 2 1 1 2	
3.463E-02	5.964E+00	20	D041	1 0 0 0 0	
4.149E-02	7.145E+00	20	F073	1 2 2 2 2	
2.903E-02	5.000E+00	20	F300	1 0 0 0 0	
3.020E-02	5.200E+00	20	S147	1 2 2 2 2	hydrate
3.693E-02	6.359E+00	23	K034	2 2 2 2 1	
3.979E-02	6.853E+00	24	K034	2 2 2 2 1	
3.484E-02	6.000E+00	25	B147	1 2 1 1 2	
4.855E-02	8.360E+00	25	C102	2 0 2 2 2	
4.550E-02	7.835E+00	25	M116	2 1 1 1 2	
4.274E-02	7.360E+00	25	M440	0 0 0 0 0	
4.820E-02	8.300E+00	25	P015	0 0 0 0 0	
4.216E-02	7.260E+00	25	S147	1 2 2 2 2	hydrate
4.437E-02	7.641E+00	26	K034	2 2 2 2 1	
4.723E-02	8.133E+00	27	K034	2 2 2 2 1	
5.008E-02	8.625E+00	28	K034	2 2 2 2 1	
4.762E-02	8.200E+00	30	B147	1 2 1 1 2	
5.633E-02	9.700E+00	30	S147	1 2 2 2 2	hydrate
5.806E-02	9.999E+00	30.5	K034	2 2 2 2 2	
6.318E-02	1.088E+01	31	A047	1 0 0 0 0	
6.205E-02	1.068E+01	31.7	K034	2 2 2 2 2	
6.829E-02	1.176E+01	33	K034	2 2 2 2 2	
7.282E-02	1.254E+01	34	K034	2 2 2 2 2	
6.388E-02	1.100E+01	35	B147	1 2 1 1 2	
7.543E-02	1.299E+01	35	S147	1 2 2 2 2	β form
7.848E-02	1.351E+01	35.5	K034	2 2 2 2 2	
1.259E-01	2.168E+01	37	A028	1 0 2 1 2	intrinsic
7.375E-02	1.270E+01	37	B147	1 2 1 1 2	
8.478E-02	1.460E+01	37	C102	2 0 2 2 2	
8.594E-02	1.480E+01	37	D084	1 0 1 0 2	
8.018E-02	1.381E+01	37	F072	1 0 0 0 2	
8.710E-02	1.500E+01	37	F300	1 0 0 0 1	
8.920E-02	1.536E+01	37	G028	2 2 1 1 2	δ form, recrystallized

(continued)

792. C₆H₈N₂O₂S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.070E-02	1.562E+01	37	G028	2 2 1 1 2	β form, recrystallized
9.120E-02	1.571E+01	37	G028	2 2 1 1 2	α form, recrystallized
9.240E-02	1.591E+01	37	G028	2 2 1 1 2	γ form
8.413E-02	1.449E+01	37	K034	2 2 2 2 2	
8.652E-02	1.490E+01	37	K086	1 0 0 0 2	
8.210E-02	1.414E+01	37	K095	2 0 0 0 2	intrinsic
8.710E-02	1.500E+01	37	L091	1 0 0 0 2	pH 5.5
8.469E-02	1.458E+01	37.50	M142	1 0 0 0 2	
9.201E-02	1.584E+01	39	K034	2 2 2 2 2	
8.362E-02	1.440E+01	40	B147	1 2 1 1 2	form II
9.750E-02	1.679E+01	40	G028	2 2 1 1 2	α form, recrystallized
9.640E-02	1.660E+01	40	G028	2 2 1 1 2	γ form
9.640E-02	1.660E+01	40	G028	2 2 1 1 2	δ form, recrystallized
9.680E-02	1.667E+01	40	G028	2 2 1 1 2	β form, recrystallized
9.518E-02	1.639E+01	40	S147	1 2 2 2 2	β form
1.049E-01	1.807E+01	42	K034	2 2 2 2 2	
1.086E-01	1.870E+01	45	B147	1 2 1 1 2	form II
1.201E-01	2.069E+01	45	S147	1 2 2 2 2	β form
1.256E-01	2.162E+01	46	K034	2 2 2 2 2	
1.527E-01	2.629E+01	50	A047	1 0 0 0 0	EFG
1.388E-01	2.390E+01	50	B147	1 2 1 1 2	form II
1.433E-01	2.468E+01	50	G028	2 2 1 1 2	δ form, recrystallized
1.419E-01	2.444E+01	50	G028	2 2 1 1 2	β form, recrystallized
1.430E-01	2.463E+01	50	G028	2 2 1 1 2	γ form
1.435E-01	2.471E+01	50	G028	2 2 1 1 2	α form, recrystallized
1.516E-01	2.610E+01	50	K034	2 2 2 2 2	
1.488E-01	2.562E+01	50	S147	1 2 2 2 2	β form
1.789E-01	3.080E+01	55	B147	1 2 1 1 2	form II
2.294E-01	3.950E+01	60	B147	1 2 1 1 2	form II
2.923E-01	5.033E+01	65	A047	1 0 0 0 0	EFG
2.962E-01	5.100E+01	65	B147	1 2 1 1 2	form II
3.833E-01	6.600E+01	70	B147	1 2 1 1 2	form II
4.599E-01	7.919E+01	75	A047	1 0 0 0 0	EFG
5.168E-01	8.900E+01	75	B147	1 2 1 1 2	form II
5.660E-01	9.747E+01	79	A047	1 0 0 0 0	EFG
6.272E-02	1.080E+01	ns	D035	0 0 0 0 2	
3.050E-02	5.252E+00	ns	L044	0 0 0 0 2	
4.571E-02	7.871E+00	ns	R427	0 0 0 0 0	
4.365E-02	7.517E+00	ns	R428	0 0 0 0 0	

793. C₆H₈N₂O₂S.H₂O

Sulfanilamide (monohydrate)

4-Aminobenzenesulfonamide (monohydrate)

p-Anilinesulfonamide (monohydrate)

Bacteramid (monohydrate)

RN: 20203-81-0 **MP (°C):****MW:** 190.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-02	4.185E+00	15	G028	2 2 1 1 2	
4.320E-02	8.218E+00	26	G028	2 2 1 1 2	
5.600E-02	1.065E+01	30	G028	2 2 1 1 2	
8.420E-02	1.602E+01	37	G028	2 2 1 1 2	

794. C₆H₈N₂O₃

5,5-Dimethylbarbituric acid

5,5-Dimethylbarbitursaeure

Barbituric acid, 5,5-dimethyl

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-dimethyl

5,5-Dimethyl barbituric acid

5,5-Dimethylbarbiturate

RN: 24448-94-0 **MP (°C):** 278**MW:** 156.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.812E-02	2.829E+00	25	P350	0 0 0 0 0	
1.549E-02	2.419E+00	ns	T003	0 0 0 0 2	intrinsic

795. C₆H₈N₂O₃S

4-Phenylhydrazine sulfonic acid

Phenylhydrazin-sulfosaeure-(4)

RN: 98-71-5 **MP (°C):****MW:** 188.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.029E-02	5.700E+00	11.50	F300	1 0 0 0 1	
1.860E-01	3.500E+01	100	F300	1 0 0 0 1	

796. C₆H₈N₂O₈

Isosorbide dinitrate

1,4:3,6-Dianhydro-D-glucitol dinitrate

Sorbidin

Isogen

Imdur

RN: 87-33-2**MP (°C):** 70**MW:** 236.14**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.328E-03	5.497E-01	25	L033	1 0 2 1 2	

797. C₆H₈N₄O

5-Amino-4-carboxymethylaminopyrimidine

RN: MP (°C):**MW:** 152.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.120E-01	3.226E+01	100	A082	1 2 0 0 0	

798. C₆H₈N₈

2,4,6,7-Tetraaminopteridine

2:4:6:7-Tetraaminopteridine

RN: 19167-63-6 **MP (°C):****MW:** 192.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.002E-04	7.692E-02	20	A020	1 2 0 1 1	

799. C₆H₈O₂

Sorbic acid

2,4-Hexadienoic acid

2-Propenylacrylic acid

Preservastat

Hexadienoic acid

Sorbistat

RN: 110-44-1 **MP (°C):** 134.5**MW:** 112.13 **BP (°C):** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	1.906E+00	30	L069	1 0 1 1 0	EFG

800. C₆H₈O₆

Tricarballylic acid

Tricarballylsaeure

1,2,3-Propanetricarboxylic acid

RN: 99-14-9 MP (°C): 166

MW: 176.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.885E+00	3.320E+02	18	F300	1 0 0 0 2	

801. C₆H₈O₆

Ascorbic acid

L-Ascorbic acid

L-Ascorbinsaeure

RN: 50-81-7 MP (°C): 193

MW: 176.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.269E-01	1.633E+02	6.99	A341	0 0 0 0 0	
9.509E-01	1.675E+02	7.99	A341	0 0 0 0 0	
9.880E-01	1.740E+02	9.99	A341	0 0 0 0 0	
1.026E+00	1.807E+02	11.99	A341	0 0 0 0 0	
1.142E+00	2.011E+02	15.99	A341	0 0 0 0 0	
1.418E+00	2.498E+02	20	D041	1 0 0 0 2	
1.254E+00	2.208E+02	20	S472	0 0 0 0 0	
1.283E+00	2.260E+02	20.99	A341	0 0 0 0 0	
1.397E+00	2.460E+02	24.99	A341	0 0 0 0 0	
1.891E+00	3.330E+02	25	D315	0 0 0 0 0	
9.757E-01	1.718E+02	25	N003	0 0 0 0 0	
1.388E+00	2.445E+02	25	S472	0 0 0 0 0	
1.551E+00	2.731E+02	28.99	A341	0 0 0 0 0	
1.533E+00	2.699E+02	30	S472	0 0 0 0 0	
1.718E+00	3.025E+02	33.99	A341	0 0 0 0 0	
1.703E+00	2.999E+02	35	S472	0 0 0 0 0	
1.758E+00	3.096E+02	35.99	A341	0 0 0 0 0	
1.856E+00	3.270E+02	38.99	A341	0 0 0 0 0	
1.028E+00	1.810E+02	40	N003	0 0 0 0 0	
1.874E+00	3.301E+02	40	S472	0 0 0 0 0	
2.009E+00	3.539E+02	42.99	A341	0 0 0 0 0	
2.021E+00	3.560E+02	43.99	A341	0 0 0 0 0	
2.066E+00	3.638E+02	44.99	A341	0 0 0 0 0	
2.054E+00	3.618E+02	45	S472	0 0 0 0 0	
2.132E+00	3.755E+02	47.69	A341	0 0 0 0 0	
2.184E+00	3.847E+02	48.49	A341	0 0 0 0 0	
2.235E+00	3.937E+02	49.99	A341	0 0 0 0 0	
2.235E+00	3.936E+02	50	S472	0 0 0 0 0	
2.255E+00	3.972E+02	50.39	A341	0 0 0 0 0	
2.275E+00	4.007E+02	50.99	A341	0 0 0 0 0	
2.373E+00	4.180E+02	52.49	A341	0 0 0 0 0	

(continued)

801. C₆H₈O₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.383E+00	4.197E+02	53.99	A341	0 0 0 0 0	
2.413E+00	4.249E+02	54.09	A341	0 0 0 0 0	
2.449E+00	4.314E+02	54.99	A341	0 0 0 0 0	
2.520E+00	4.439E+02	60.02	A341	0 0 0 0 0	
2.551E+00	4.492E+02	61.99	A341	0 0 0 0 0	
2.635E+00	4.641E+02	64.99	A341	0 0 0 0 0	
1.891E+00	3.330E+02	ns	M054	0 0 0 0 2	

802. C₆H₈O₇

Citric acid anhydrous

2-Hydroxytricarballylic acid

Citronensaeure

1,2,3-Propanetricarboxylic acid

Citro

Citralite

RN: 77-92-9 MP (°C): 153
 MW: 192.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.549E+00	4.898E+02	0	M043	1 0 0 0 1	
1.881E+00	3.613E+02	1.2	K084	1 0 1 0 2	
1.875E+00	3.602E+02	1.6	K084	1 0 1 0 2	
2.562E+00	4.923E+02	4.99	A339	0 0 0 0 0	
1.825E+00	3.506E+02	10	D020	1 2 1 1 2	
2.571E+00	4.940E+02	10	F300	1 0 0 0 2	
1.825E+00	3.506E+02	10	F302	1 0 0 0 1	
2.817E+00	5.413E+02	10	M043	1 0 0 0 2	
1.938E+00	3.723E+02	10.0	K084	1 0 1 0 2	
2.684E+00	5.157E+02	9.99	A339	0 0 0 0 0	
1.927E+00	3.702E+02	10.8	K084	1 0 1 0 2	
2.811E+00	5.400E+02	14.99	A339	0 0 0 0 0	
1.933E+00	3.713E+02	15.0	K084	1 0 1 0 2	
2.918E+00	5.605E+02	19.99	A339	0 0 0 0 0	
3.089E+00	5.935E+02	20	D041	1 0 0 0 2	
2.816E+00	5.410E+02	20	F300	1 0 0 0 2	
1.935E+00	3.719E+02	20	F302	1 0 0 0 2	
3.089E+00	5.935E+02	20	M043	1 0 0 0 2	
3.045E+00	5.851E+02	24.99	A339	0 0 0 0 0	
1.994E+00	3.831E+02	25	D020	1 2 1 1 2	
1.254E+01	2.409E+03	25	K040	1 0 2 1 2	
3.201E+00	6.149E+02	29.99	A339	0 0 0 0 0	
2.037E+00	3.914E+02	30	F302	1 0 0 0 2	
3.366E+00	6.466E+02	30	M043	1 0 0 0 2	
3.296E+00	6.332E+02	34.99	A339	0 0 0 0 0	
2.100E+00	4.034E+02	35.8	D039	2 2 1 2 2	EFG
2.094E+00	4.023E+02	36.6	F302	1 0 0 0 2	
3.201E+00	6.150E+02	36.60	F300	1 0 0 0 2	

(continued)

802. C₆H₈O₇ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.346E+00	6.429E+02	39.99	A339	0 0 0 0 0	
2.118E+00	4.069E+02	40	D020	1 2 1 1 2	
2.116E+00	4.065E+02	40	D039	2 2 1 2 0	EFG
2.118E+00	4.069E+02	40	F302	1 0 0 0 2	
3.553E+00	6.825E+02	40	M043	1 0 0 0 2	
3.438E+00	6.605E+02	44.99	A339	0 0 0 0 0	
3.488E+00	6.702E+02	49.99	A339	0 0 0 0 0	
2.161E+00	4.152E+02	50	D039	2 2 1 2 0	EFG
2.159E+00	4.149E+02	50	F302	1 0 0 0 2	
3.539E+00	6.800E+02	54.99	A339	0 0 0 0 0	
3.601E+00	6.918E+02	59.99	A339	0 0 0 0 0	
2.214E+00	4.253E+02	60	D039	2 2 1 2 0	EFG
2.205E+00	4.236E+02	60	F302	1 0 0 0 2	
3.824E+00	7.347E+02	60	M043	1 0 0 0 2	
3.669E+00	7.050E+02	64.99	A339	0 0 0 0 0	
2.261E+00	4.344E+02	70	D039	2 2 1 2 0	EFG
2.251E+00	4.325E+02	70	F302	1 0 0 0 2	
2.300E+00	4.420E+02	80	D039	2 2 1 2 0	EFG
2.294E+00	4.407E+02	80	F302	1 0 0 0 2	
4.102E+00	7.881E+02	80	M043	1 0 0 0 2	
2.350E+00	4.515E+02	90	D039	2 2 1 2 0	EFG
2.336E+00	4.487E+02	90	F302	1 0 0 0 2	
2.391E+00	4.595E+02	100	D039	2 2 1 2 0	EFG
4.372E+00	8.400E+02	100	D041	1 0 0 0 2	
3.997E+00	7.680E+02	100	F300	1 0 0 0 2	
2.376E+00	4.565E+02	100	F302	1 0 0 0 1	
4.373E+00	8.403E+02	100	M043	1 0 0 0 2	
1.885E+00	3.621E+02	.0	K084	1 0 1 0 2	

803. C₆H₈O₇·H₂O

Citric acid (monohydrate)

2-Hydroxytricarballylic acid (monohydrate)

RN: 5949-29-1 MP (°C):

MW: 210.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E+00	3.266E+02	0	D039	2 2 1 2 0	EFG
1.667E+00	3.502E+02	10	D039	2 2 1 2 0	EFG
3.005E+00	6.314E+02	17.20	L031	1 1 2 1 2	average of 2
3.077E+00	6.466E+02	19.80	L031	1 1 2 1 2	
1.771E+00	3.723E+02	20	D039	2 2 1 2 0	EFG
3.080E+00	6.473E+02	20.20	L031	1 1 2 1 2	
3.146E+00	6.610E+02	22.50	L031	1 1 2 1 2	
3.154E+00	6.627E+02	22.90	L031	1 1 2 1 2	
1.822E+00	3.830E+02	25	D039	2 2 1 2 2	EFG
3.214E+00	6.753E+02	25.10	L031	1 1 2 1 2	
3.216E+00	6.759E+02	25.30	L031	1 1 2 1 2	

(continued)

803. C₆H₈O₇.H₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.272E+00	6.875E+02	27.00	L031	1 1 2 1 2	
3.276E+00	6.885E+02	27.60	L031	1 1 2 1 2	
3.303E+00	6.942E+02	28.60	L031	1 1 2 1 2	
1.864E+00	3.917E+02	30	D039	2 2 1 2 0	EFG
3.359E+00	7.059E+02	30.50	L031	1 1 2 1 2	
3.357E+00	7.054E+02	30.70	L031	1 1 2 1 2	
3.389E+00	7.122E+02	31.80	L031	1 1 2 1 2	
3.440E+00	7.230E+02	33.70	L031	1 1 2 1 2	
3.478E+00	7.308E+02	34.40	L031	1 1 2 1 2	
3.518E+00	7.392E+02	35.40	L031	1 1 2 1 2	

804. C₆H₈S

2-Ethylthiophene

Thiophene, 2-ethyl-

RN: 872-55-9

MP (°C): <25

MW: 112.19

BP (°C): 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.603E-03	2.920E-01	25	K119	1 0 0 0 2	
2.603E-03	2.920E-01	25	P051	2 1 1 2 2	
2.603E-03	2.920E-01	25.00	P007	2 1 2 2 2	

805. C₆H₉ClO₃

Ethyl 2-chloroacetocetate

2-Chloroacetoacetic acid ethyl ester

RN: 609-15-4

MP (°C):

MW: 164.59

BP (°C): 107 at 14 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.407E-02	8.900E+00	30	B433	0 0 0 0 0	

806. C₆H₉NO₃

4,6,10-Trioxa-1-azatricyclo[3.3.1.13,7]decane

Trimorpholin

Trimorpholine

RN: 281-36-7

MP (°C):

MW: 143.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E+00	1.670E+02	0	F300	1 0 0 0 2	
2.375E+00	3.400E+02	80	F300	1 0 0 0 2	

807. C₆H₉NO₃

Trimethadione

3,5,5-Trimethyl-2,4-diketooxazolidine

3,5,5-Trimethyl-2,4-oxazolidinedione

Tridione

RN: 127-48-0 **MP (°C):** 46**MW:** 143.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.327E-01	4.762E+01	20	D041	1 0 0 0 0	

808. C₆H₉NO₆

Triglycine

Complexon I

N,N-bis(Carboxymethyl)glycine

α,α',α²-Trimethylaminetricarboxylic acid**RN:** 139-13-9 **MP (°C):** 241.5**MW:** 191.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.090E-01	5.906E+01	25	M024	1 2 0 1 2	
3.395E-01	6.490E+01	25.1	N024	0 0 0 0 0	
3.374E-01	6.450E+01	25.1	N025	0 0 0 0 0	
3.348E-01	6.400E+01	25.1	N026	0 0 0 0 0	
3.101E-01	5.927E+01	25.1	N027	1 2 2 2 2	

809. C₆H₉N₃

Kyanmethin

6-Amino-2,4-dimethyl-pyrimidin

6-Amino-2,4-dimethylpyrimidine

RN: 461-98-3 **MP (°C):** 182**MW:** 123.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.197E-02	6.400E+00	18	F300	1 0 0 0 1	

810. C₆H₉N₃O₂

2-Isopropyl-4(5)-nitroimidazole

1H-Imidazole, 2-(1-methylethyl)-4-nitro-

2-(1-Methylethyl)-4-nitro-1H-imidazole

2-Isopropyl-5-nitroimidazole

2-Isopropyl-4-nitroimidazole

RN: 13373-32-5 **MP (°C):** 182–183**MW:** 155.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.025E-02	1.090E+01	20	D344	0 0 0 0 0	
7.025E-02	1.090E+01	20	D344	0 0 0 0 0	
6.886E-02	1.068E+01	20	D344	0 0 0 0 0	
7.030E-02	1.091E+01	20	D344	0 0 0 0 0	

811. C₆H₉N₃O₂

L-Histidine

L-Histidin

Histidine

RN: 71-00-1 **MP (°C):** 287**MW:** 155.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.580E-01	4.003E+01	15	D349	2 1 1 2 2	
2.646E-01	4.106E+01	20	B032	1 2 2 1 2	
2.640E-01	4.096E+01	20	D349	2 1 1 2 2	
2.930E-01	4.546E+01	25	B032	1 2 2 1 2	
2.574E-01	3.994E+01	25	D041	1 0 0 0 2	
2.720E-01	4.220E+01	25	D349	2 1 1 2 2	
2.481E-01	3.850E+01	25	F300	1 0 0 0 2	
2.651E-01	4.114E+01	25	G315	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N024	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N025	0 0 0 0 0	
2.771E-01	4.300E+01	25.1	N026	0 0 0 0 0	
2.675E-01	4.150E+01	25.1	N027	1 1 2 2 2	
2.791E-01	4.330E+01	27	D036	0 0 0 0 0	
3.207E-01	4.976E+01	29.80	B032	1 2 2 1 2	
2.834E-01	4.398E+01	30	H062	2 2 2 0 1	EFG
5.213E-01	8.088E+01	50	H062	2 2 2 0 0	EFG
7.915E-01	1.228E+02	70	H062	2 2 2 0 0	EFG

812. C₆H₉N₃O₂

6-Amino-1,3-dimethyluracil

RN: 6642-31-5 **MP (°C):****MW:** 155.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.550E-02	7.060E+00	25	Z408	0 0 0 0 0	

813. C₆H₉N₃O₃

Metronidazole

Flagyl

2-Methyl-5-nitroimidazole-1-ethanol

Metrozine

Rozex

2-Methyl-5-nitro-1-imidazoleethanol

RN: 443-48-1 **MP (°C):** 158**MW:** 171.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.545E-02	9.490E+00	20	D344	0 0 0 0 0	
5.545E-02	9.490E+00	20	D344	0 0 0 0 0	
5.441E-02	9.312E+00	20	D344	0 0 0 0 0	
5.540E-02	9.482E+00	20	D344	0 0 0 0 0	
4.809E-02	8.232E+00	20	H324	0 0 0 0 0	
5.785E-02	9.901E+00	20	I315	0 0 0 0 0	
6.427E-02	1.100E+01	25	C062	1 1 2 1 2	
5.550E-02	9.500E+00	25	C124	2 0 1 1 2	
5.727E-02	9.803E+00	26	H324	0 0 0 0 0	
6.585E-02	1.127E+01	30	H324	0 0 0 0 0	
5.843E-02	1.000E+01	ns	C324	0 0 0 0 0	
5.843E-02	1.000E+01	ns	K444	0 0 0 0 0	

814. C₆H₁₀

1,5-Hexadiene

Biallyl

Diallyl

RN: 592-42-7 **MP (°C):** -141**MW:** 82.15 **BP (°C):** 60

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.057E-03	1.690E-01	25	M001	2 1 2 2 2	

815. C₆H₁₀

Cyclohexene

1,2,3,4-Tetrahydrobenzene

RN: 110-83-8 **MP (°C):** -104**MW:** 82.15 **BP (°C):** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.408E-03	2.799E-01	4.8	L007	2 2 1 2 2	
3.408E-03	2.799E-01	5.1	L007	2 0 1 1 2	
3.633E-03	2.984E-01	14.8	L007	2 2 1 2 2	
3.633E-03	2.984E-01	15.2	L007	2 0 1 1 2	
1.583E-03	1.300E-01	20	C008	1 2 2 0 1	
2.769E-03	2.274E-01	20	M337	2 1 2 2 2	

(continued)

815. C₆H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-03	2.834E-01	23.5	S171	2 1 2 2 2	
3.639E-03	2.989E-01	24.8	L007	2 2 1 2 2	
2.593E-03	2.130E-01	25	M001	2 1 2 2 2	
3.639E-03	2.989E-01	25.1	L007	2 0 1 1 2	
3.681E-03	3.024E-01	34.8	L007	2 2 1 2 2	
3.681E-03	3.024E-01	35.2	L007	2 0 1 1 2	
6.000E-03	4.929E-01	40	P335	0 0 0 0 0	
3.779E-03	3.104E-01	44.8	L007	2 2 1 2 2	
3.779E-03	3.104E-01	45.2	L007	2 0 1 1 2	
1.800E-02	1.479E+00	140	P335	0 0 0 0 0	
1.583E-03	1.300E-01	ns	M010	0 0 0 0 1	

816. C₆H₁₀

1-Hexyne

Butylacetylene

n-Butylacetylene

RN: 693-02-7 **MP (°C):** -132
MW: 82.15 **BP (°C):** 71

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.382E-03	3.600E-01	25	M001	2 1 2 2 2	
8.370E-03	6.876E-01	25	M342	1 0 1 1 2	

817. C₆H₁₀

3-Hexyne

Diethylacetylene

RN: 928-49-4 **MP (°C):** -103
MW: 82.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	5.586E-01	25	H039	1 2 2 2 1	
6.400E-03	5.257E-01	35	H039	1 2 2 2 1	

818. C₆H₁₀BrNO₄

5-Bromo-2-ethyl-5-nitro-1,3-dioxane

2-Ethyl-5-bromo-5-nitro-1,3-dioxane

RN: 54010-85-4 **MP (°C):** 58-59
MW: 240.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.205E-03	7.694E-01	25	L013	1 0 2 1 2	

819. C₆H₁₀BrNO₄

5-Bromo-2,2-dimethyl-5-nitro-1,3-dioxane

2,2-Dimethyl-5-bromo-5-nitro-1,3-dioxane

m-Dioxane, 5-bromo-2,2-dimethyl-5-nitro-

RN: 60766-57-6 MP (°C): 79–81

MW: 240.06 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.369E-03	1.049E+00	25	L013	1 0 2 1 2	

820. C₆H₁₀ClN₅

Deethylatrazine

2-Amino-4-isopropylamino-6-chloro-s-triazine

6-Chloro-N-(1-methylethyl)-1,3,5-triazine-2,4-diamine

RN: 6190-65-4 MP (°C):

MW: 187.63 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	3.753E-01	2	B193	1 1 0 0 1	

821. C₆H₁₀O

Mesityl oxide

Mesityloxid

RN: 141-79-7 MP (°C): -57

MW: 98.15 BP (°C): 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.862E-01	2.809E+01	20	D052	1 1 0 0 0	
2.975E-01	2.920E+01	ns	F300	0 0 0 0 2	

822. C₆H₁₀O

Cyclohexanone

Cyclohexanon

RN: 108-94-1 MP (°C): -47

MW: 98.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-02	1.298E+00	20	D052	1 1 0 0 1	sic
2.485E-01	2.439E+01	25	B060	2 0 1 1 1	
8.975E-01	8.809E+01	25	M323	2 2 1 1 2	

823. C₆H₁₀OS₂

Allicin

2-Propene-1-sulfinothioic acid S-2-propenyl ester

RN: 539-86-6 MP (°C): <25

MW: 162.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.479E-01	2.400E+01	10	F300	1 0 0 0 1	

824. C₆H₁₀O₂

Methyl vinyl carbinol acetate

1-Methylallyl acetate

3-Buten-2-yl acetate

RN: 6737-11-7 MP (°C):

MW: 114.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-01	1.303E+01	26	O012	1 2 1 1 2	
6.953E-02	7.937E+00	50	O012	1 2 1 1 2	
1.718E-01	1.961E+01	75	O012	1 2 1 1 2	

825. C₆H₁₀O₂

3-Methyl-1,3-pentadione

1,2-Dimethyl-1,3-butadiene

3,4-Dimethylbutadiene

RN: 4549-74-0 MP (°C): -5

MW: 114.15 BP (°C): 191

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.780E-01	1.116E+02	25	M078	2 0 1 0 2	

826. C₆H₁₀O₂S₄

Dixanthogen

Ethyl dixanthogen

RN: 502-55-6 MP (°C): 28

MW: 242.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-05	3.151E-03	22	P076	1 2 1 1 1	
1.140E-05	2.763E-03	25	H102	1 2 1 2 2	
<2.06E-06	<5.00E-04	25	M161	1 0 0 0 0	
1.250E-05	3.030E-03	ns	L083	0 0 0 0 0	EFG, pH 3-9

827. C₆H₁₀O₃

Ethyl acetoacetate

Acetessigsaeure-aethyl ester

Acetoacetic acid ethyl ester

RN: 141-97-9 **MP (°C):** -45
MW: 130.14 **BP (°C):** 180.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.613E-01	1.251E+02	10.5	D041	1 0 0 0 2	
8.529E-01	1.110E+02	16.50	F300	1 0 0 0 2	

828. C₆H₁₀O₄

2,2-Dimethylsuccinic acid

α,α-Dimethylbernsteinsaeure

RN: 597-43-3 **MP (°C):** 140.5
MW: 146.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.790E-01	7.000E+01	14	F300	1 0 0 0 2	

829. C₆H₁₀O₄

sym-Dimethylsuccinic acid

Acide Dimethylsuccinique-sym

RN: 608-40-2 **MP (°C):**
MW: 146.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E+00	3.000E+02	15	M051	1 0 0 0 2	

830. C₆H₁₀O₄

n-Propylmalonic acid

Acide n-propylmalonique

RN: 616-62-6 **MP (°C):**
MW: 146.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E+00	4.560E+02	0	M051	1 0 0 0 2	
4.112E+00	6.010E+02	15	M051	1 0 0 0 2	
4.790E+00	7.000E+02	25	M051	1 0 0 0 2	
6.459E+00	9.440E+02	50	M051	1 0 0 0 2	

831. C₆H₁₀O₄

Ethylene glycol diacetate

Glycol diacetate

RN: 111-55-7 **MP (°C):** -31
MW: 146.14 **BP (°C):** 190

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E+00	1.756E+02	20	D052	1 1 0 0 2	
9.661E-01	1.412E+02	20	M062	1 0 0 0 2	
8.526E-01	1.246E+02	22	F300	1 0 0 0 2	
1.034E+00	1.511E+02	24.50	O005	2 0 2 2 2	
1.070E+00	1.564E+02	25	F064	1 0 0 0 2	
1.220E-01	1.783E+01	ns	F014	0 0 0 0 2	

832. C₆H₁₀O₄

DL-2,3-Dimethylsuccinic acid

DL- α , α' -Dimethylbernsteinsaeure

RN: 13545-04-5 **MP (°C):** 120
MW: 146.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E-01	3.000E+01	14	F300	1 0 0 0 0	

833. C₆H₁₀O₄

Adipic acid

Adipinsaeure

RN: 124-04-9 **MP (°C):** 152
MW: 146.14 **BP (°C):** 337.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.431E-02	7.937E+00	0	M043	1 0 0 0 0	
6.766E-02	9.888E+00	4.99	A339	0 0 0 0 0	
6.775E-02	9.901E+00	10	M043	1 0 0 0 1	
7.853E-02	1.148E+01	9.99	A339	0 0 0 0 0	
1.061E-01	1.551E+01	14.99	A339	0 0 0 0 0	
9.580E-02	1.400E+01	15	F300	1 0 0 0 1	
9.580E-02	1.400E+01	15	L041	1 0 0 1 1	
9.580E-02	1.400E+01	15	M051	1 0 0 0 1	
1.303E-01	1.904E+01	19.99	A339	0 0 0 0 0	
1.011E-01	1.478E+01	20	D041	1 0 0 0 1	
1.276E-01	1.865E+01	20	M043	1 0 0 0 1	
9.856E-02	1.440E+01	20	M171	1 0 0 0 1	
9.000E-02	1.315E+01	20	S006	1 0 0 0 1	
4.824E-01	7.050E+01	21	B040	1 0 1 1 2	sic
1.664E-01	2.432E+01	24.99	A339	0 0 0 0 0	
2.216E-03	3.239E-01	25	K035	2 0 0 0 2	sic
2.053E-01	3.001E+01	29.99	A339	0 0 0 0 0	

(continued)

833. C₆H₁₀O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.993E-01	2.913E+01	30	M043	1 0 0 0 1	
2.045E-01	2.988E+01	34.10	A031	1 2 2 2 2	
2.546E-01	3.721E+01	34.99	A339	0 0 0 0 0	
2.933E-01	4.287E+01	39.3	G302	2 2 2 2 0	EFG
3.274E-01	4.785E+01	39.99	A339	0 0 0 0 0	
3.333E-01	4.871E+01	40	A031	1 2 2 2 2	
3.382E-01	4.943E+01	40	B088	1 0 0 0 1	
3.258E-01	4.762E+01	40	M043	1 0 0 0 1	
4.383E-01	6.406E+01	44.99	A339	0 0 0 0 0	
5.516E-01	8.062E+01	49.99	A339	0 0 0 0 0	
5.788E-01	8.458E+01	50	A031	1 2 2 2 2	
7.508E-01	1.097E+02	54.99	A339	0 0 0 0 0	
1.011E+00	1.477E+02	59.99	A339	0 0 0 0 0	
1.024E+00	1.497E+02	60	A031	1 2 2 2 2	
1.044E+00	1.525E+02	60	M043	1 0 0 0 1	
1.130E+00	1.652E+02	64.99	A339	0 0 0 0 0	
1.740E+00	2.543E+02	70	A031	1 2 2 2 2	
2.818E+00	4.118E+02	80	M043	1 0 0 0 1	
3.330E+00	4.867E+02	87.10	A031	1 2 2 2 2	
4.277E+00	6.250E+02	100	F300	1 0 0 0 2	
4.211E+00	6.154E+02	100	M043	1 0 0 0 2	
1.662E-01	2.430E+01	rt	H431	0 0 0 0 0	

834. C₆H₁₀O₄Methyl α -acetoxypropionate

Methyl 2-acetoxypropionate

Methyl *O*-acetylactate

Methyl 2-acetoxypropanoate

RN: 6284-75-9 MP (°C):

MW: 146.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.556E-01	8.120E+01	25	R006	2 2 0 1 2	

835. C₆H₁₀O₅

Propanoic acid, 2-[(methoxycarbonyl)oxy]-, methyl ester

Carbonic acid, methyl ester, ester with methyl lactate

RN: 6288-11-5 MP (°C):

MW: 162.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-01	3.911E+01	25	R007	0 0 0 0 0	

836. C₆H₁₀O₈

D-Talogalactaric acid

D-Taloschleimsaeure

D-Galactaric acid

Galactaric acid

Schleimsaeure

RN: 526-99-8 MP (°C): > 230

MW: 210.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	3.289E+00	14	D041	1 0 0 0 1	
1.570E-02	3.300E+00	14	F300	1 0 0 0 1	
8.090E-02	1.700E+01	100	F300	1 0 0 0 1	

837. C₆H₁₁Br

Bromocyclohexane

Cyclohexyl bromide

RN: 108-85-0 MP (°C):

MW: 163.06 BP (°C): 166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.012E-03	8.173E-01	ns	S460	0 0 0 0 0	

838. C₆H₁₁BrN₂O₂

α-Methyl-γ-bromo-butanoic ureide

RN: MP (°C):

MW: 223.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.658E-02	1.039E+01	ns	F056	0 2 2 2 1	

839. C₆H₁₁BrN₂O₂

α-Bromo-isovaleric ureide

Butanamide, *N*-(aminocarbonyl)-2-bromo-3-methyl-

Dormigene

Pivadorn

Pivadorm

Isobromyl

RN: 496-67-3 MP (°C):

MW: 223.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.531E-02	1.903E+01	ns	F057	0 2 2 2 2	

840. C₆H₁₁BrN₂O₂

3-Bromo-2-methyl-butanoic ureide

Urea, (2-bromo-2-methylbutyryl)-

DL-*N*-(2-Bromo-2-methylbutanoyl)urea**RN:** 14368-76-4 **MP (°C):****MW:** 223.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-01	3.101E+01	ns	F056	0 2 2 2 1	

841. C₆H₁₁BrN₂O₂

β-Bromo-valeric acid ureide

RN: **MP (°C):****MW:** 223.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.470E-02	7.740E+00	ns	F056	0 2 2 2 1	

842. C₆H₁₁BrN₂O₂

γ-Bromo-valeric acid ureide

RN: **MP (°C):****MW:** 223.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.307E-02	9.607E+00	ns	F056	0 2 2 2 1	

843. C₆H₁₁BrN₂O₂

α-Bromo-valeric acid ureide

Pentanamide, *N*-(aminocarbonyl)-2-bromo-**RN:** 66947-87-3 **MP (°C):****MW:** 223.08 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.690E-02	8.232E+00	ns	F056	0 2 2 2 1	
3.703E-02	8.261E+00	ns	F057	0 2 2 2 2	

844. C₆H₁₁NO

Caprolactam

ε-Caprolactam

RN: 105-60-2 **MP (°C):** 70**MW:** 113.16 **BP (°C):** 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.776E+00	4.273E+02	5.70	B201	2 2 2 1 2	
3.850E+00	4.357E+02	10.30	B201	2 2 2 1 2	

845. C₆H₁₁NO

Cyclohexanone oxime

Antioxidant D

(Hydroxyimino)cyclohexane

RN: 100-64-1 **MP (°C):** 90
MW: 113.16 **BP (°C):** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.409E-01	1.594E+01	25.5	K087	1 0 0 0 2	
1.580E-01	1.787E+01	32.0	K087	1 0 0 0 2	
1.648E-01	1.865E+01	36.8	K087	1 0 0 0 2	
1.936E-01	2.191E+01	44.0	K087	1 0 0 0 2	
2.155E-01	2.439E+01	48.8	K087	1 0 0 0 2	
2.715E-01	3.073E+01	60.4	K087	1 0 0 0 2	
2.922E-01	3.307E+01	63.7	K087	1 0 0 0 2	
3.194E-01	3.614E+01	76.2	K087	1 0 0 0 2	
3.456E-01	3.911E+01	83.1	K087	1 0 0 0 2	
4.039E-01	4.571E+01	95.2	K087	1 0 0 0 2	
4.939E-01	5.589E+01	110.7	K087	1 0 0 0 2	
5.743E-01	6.498E+01	120	K087	1 0 0 0 2	
7.386E-01	8.358E+01	131	K087	1 0 0 0 2	

846. C₆H₁₁NO₂S

2,2-Dimethylthiazolidine-4-carboxylic acid

4-Thiazolidinecarboxylic acid, 2,2-dimethyl-
Thiazolidine-4-carboxylic acid, 2,2-dimethyl-

RN: 42607-20-5 **MP (°C):**
MW: 161.22 **BP (°C):** 317.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-01	4.837E+01	21	B414	1 0 0 1 1	very fast and extent decomposition, uncertain value

847. C₆H₁₁NO₄

α-Aminoadipic acid

2-Aminohexanedioic acid

α-Amino-adipinsaeure

RN: 542-32-5 **MP (°C):**
MW: 161.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.365E-02	2.200E+00	20	F300	1 0 0 0 1	

848. C₆H₁₁NO₄

Glycine, *N*-(carboxymethyl)-, 1-ethyl ester
AcGlyOEt

Acetic acid, iminodi-, monoethyl ester

RN: 21885-31-4 **MP (°C):**

MW: 161.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.074E-03	1.140E+00	27	D036	0 0 0 0 0	

849. C₆H₁₁N₂O₄PS₃

Methidathion

Supracide

S-((5-Methoxy-2-oxo-1,3,4-thiadiazol-3(2H)-yl)methyl) *O,O*-dimethyl phosphorodithioate

Ultracide

Somanil

S-2,3-Dihydro-5-methoxy-2-oxo-1,3,4-thiadiazol-3-ylmethyl *O,O*-dimethylphosphorodithioate

RN: 950-37-8 **MP (°C):**

MW: 302.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.186E-04	1.870E-01	20	B300	2 2 1 1 2	
8.269E-04	2.500E-01	20	F311	1 2 2 2 1	
7.938E-04	2.400E-01	25	M161	1 0 0 0 2	

850. C₆H₁₁N₃O₆

Glycine tripeptide

RN: **MP (°C):**

MW: 221.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.127E-01	4.705E+01	20	B032	1 2 2 1 2	
2.907E-01	6.430E+01	25	B032	1 2 2 1 2	
3.565E-01	7.884E+01	29.80	B032	1 2 2 1 2	

851. C₆H₁₂

Methylcyclopentane

MCP

RN: 96-37-7 **MP (°C):** -142

MW: 84.16 **BP (°C):** 72

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.967E-04	4.180E-02	25	K119	1 0 0 0 2	
4.990E-04	4.200E-02	25	M001	2 1 2 2 2	
5.062E-04	4.260E-02	25	M002	2 1 2 2 2	

(continued)

851. C₆H₁₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.967E-04	4.180E-02	25	P051	2 1 1 2 2	
4.967E-04	4.180E-02	25.00	P007	2 1 2 2 2	
4.990E-04	4.200E-02	ns	H123	0 0 0 0 0	

852. C₆H₁₂

Cyclohexane

Cyclohexan

RN: 110-82-7

MP (°C): 7

MW: 84.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.734E-04	8.192E-02	4.8	L007	2 1 1 2 2	
9.734E-04	8.192E-02	5.1	L007	2 0 1 1 2	
1.054E-03	8.869E-02	14.8	L007	2 1 1 2 2	
1.054E-03	8.869E-02	15.2	L007	2 0 1 1 2	
9.505E-04	8.000E-02	16	D047	1 0 0 1 1	
<5.94E-04	<5.00E-02	17	F300	1 0 0 0 0	
4.396E-04	3.700E-02	20	M337	2 1 2 2 2	
6.178E-04	5.200E-02	23.5	S171	2 1 2 2 2	
1.055E-03	8.883E-02	24.8	L007	2 1 1 2 2	
9.505E-04	7.999E-02	25	G068	1 0 1 0 0	
6.939E-04	5.840E-02	25	G313	2 1 1 2 2	
1.426E-03	1.200E-01	25	K112	1 0 2 1 1	
7.901E-04	6.650E-02	25	K119	1 0 0 0 2	
6.737E-04	5.670E-02	25	L002	2 2 2 2 2	
6.535E-04	5.500E-02	25	M001	2 1 2 2 2	
6.535E-04	5.500E-02	25	M002	2 1 2 2 2	
6.535E-04	5.500E-02	25	M040	1 0 0 1 1	
6.832E-04	5.750E-02	25	M132	2 2 2 1 2	
7.901E-04	6.650E-02	25	P051	2 1 1 2 2	
6.270E-04	5.277E-02	25	S359	2 1 2 2 2	
7.901E-04	6.650E-02	25.00	P007	2 1 2 2 2	
1.055E-03	8.883E-02	34.8	L007	2 1 1 2 2	
1.055E-03	8.883E-02	35.2	L007	2 0 1 1 2	
5.389E-04	4.535E-02	38	K055	1 2 0 1 1	
1.085E-03	9.131E-02	44.8	L007	2 1 1 2 2	
1.085E-03	9.131E-02	45.2	L007	2 0 1 1 2	
1.426E-03	1.200E-01	50	L097	1 1 1 1 1	
2.020E-03	1.700E-01	56	G068	1 0 1 0 1	
3.222E-04	2.712E-02	71	K055	1 2 0 1 1	
3.326E-03	2.799E-01	94	G068	1 0 1 0 1	
1.200E-04	1.010E-02	ns	D348	0 0 0 0 0	
6.535E-04	5.500E-02	ns	H123	0 0 0 0 0	
5.000E-03	4.208E-01	ns	H333	0 1 0 1 0	EFG
9.505E-04	8.000E-02	ns	M010	0 0 0 0 0	
6.642E-04	5.590E-02	ns	M175	0 0 2 1 2	

853. C₆H₁₂

4-Methyl-1-pentene

4-Methylpentene

Isohexene

RN: 691-37-2**MP (°C):** -154**MW:** 84.16**BP (°C):** 53

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.703E-04	4.800E-02	25	M001	2 1 2 2 1	

854. C₆H₁₂

2-Methyl-1-pentene

4-Methyl-4-pentene

RN: 763-29-1**MP (°C):** -136**MW:** 84.16**BP (°C):** 62

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.268E-04	7.800E-02	25	M001	2 1 2 2 2	

855. C₆H₁₂

1-Hexene

1-*n*-Hexene

Hexene

Dialen 6

RN: 592-41-6**MP (°C):** -140**MW:** 84.16**BP (°C):** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.822E-04	4.900E-02	23	C332	0 0 0 0 0	
6.583E-04	5.540E-02	25	L002	2 2 2 2 2	
5.941E-04	5.000E-02	25	M001	2 1 2 2 2	
5.941E-04	5.000E-02	25	M040	1 0 0 1 1	
8.280E-04	6.969E-02	25	M342	1 0 1 1 2	

856. C₆H₁₂ClNOAcetamide, 2-chloro-*N,N*-diethyl-

CDEA

RN: 2315-36-8**MP (°C):****MW:** 149.62**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.264E-01	7.877E+01	25	B185	0 0 0 0 0	

857. C₆H₁₂Cl₂O

Dichloroisopropyl ether
 bis(2-Chloro-1-methylethyl) ether
 DCIP
 β,β'-Dichlorodiisopropyl ether
 2,2'-Oxybis[1-chloropropane]
 Pichloram

RN: 63283-80-7 **MP (°C):**
MW: 171.07 **BP (°C):** 187.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.921E-03	1.697E+00	20	M062	1 0 0 0 1	

858. C₆H₁₂Cl₂O₂

1,2-bis(2-Chloroethoxy)ethane
 Triglycol dichloride

RN: 112-26-5 **MP (°C):** 121
MW: 187.07 **BP (°C):** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.916E-02	1.855E+01	20	M062	1 0 0 0 2	

859. C₆H₁₂Cl₃O₄P

tris-(2-Chloroethyl) phosphate
 Tri-β-chloroethyl phosphate

RN: 115-96-8 **MP (°C):**
MW: 285.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.01E-04	<2.00E-01	25	B070	1 2 0 1 0	

860. C₆H₁₂NO₃PS₂

Diethyl 1,3-dithietan-2-ylideneephosphoramidate
 Nematak
 AC 64475
 Geofos
 Fosthietan
 CL 64475

RN: 21548-32-3 **MP (°C):**
MW: 241.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.072E-01	5.000E+01	25	M161	1 0 0 0 1	

861. C₆H₁₂NO₄PS₂

Formothion

O,O-Dimethyl S-(*N*-methyl-*N*-formylcarbamoylmethyl) dithiophosphate**RN:** 2540-82-1 **MP (°C):****MW:** 257.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.011E-02	2.600E+00	24	M161	1 0 0 0 1	

862. C₆H₁₂N₂O*N*-Nitrosohexamethyleneimine

NHMI

RN: 932-83-2 **MP (°C):****MW:** 128.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.282E+01	24	M031	1 1 1 1 1	

863. C₆H₁₂N₂O₂

2,6-Dimethylnitrosomorpholine

DMNM

RN: 1456-28-6 **MP (°C):****MW:** 144.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.600E-01	1.240E+02	24	M031	1 1 1 1 1	

864. C₆H₁₂N₂O₂

Adipamide

Adipinsaeurediamid

RN: 628-94-4 **MP (°C):****MW:** 144.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.052E-02	4.400E+00	12.20	F300	1 0 0 0 1	

865. C₆H₁₂N₂O₃

Daminozide

N-Dimethylamino-β-carbamyl propionic acid

Succinic acid 2,2-dimethylhydrazide

Alar

DMASA

RN: 1596-84-5 MP (°C): 155

MW: 160.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-01	1.000E+02	25	M161	1 0 0 0 2	

866. C₆H₁₂N₂O₃

δ-Aminovaleric hydantoic acid

δ-Uramidovaleric acid

RN: MP (°C): 179

MW: 160.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.740E-02	2.787E+00	25	M024	1 2 0 1 2	

867. C₆H₁₂N₂O₃S

Methomyl

Acetamidic acid

N-[(methyl-carbamoyl)oxy]-, methyl ester

Carbamic acid

Lannabait

Nudrin

RN: 16752-77-5 MP (°C): 78

MW: 192.24 BP (°C): 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.548E-01	6.821E+01	ns	R424	0 0 0 0 0	

868. C₆H₁₂N₂O₄S₂

L-Cystine

3,3'-Dithiobis(2-aminopropanoic acid)

RN: 56-89-3 MP (°C):

MW: 240.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.021E-03	4.858E-01	20	H082	1 2 1 1 2	isomeric
7.905E-04	1.900E-01	20	H082	1 2 1 1 2	plate cystine
6.910E-04	1.660E-01	24.99	C404	2 1 2 2 1	
7.000E-02	1.682E+01	25	C405	2 1 2 2 2	intrinsic zwit

(continued)

868. C₆H₁₂N₂O₄S₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.536E-04	1.090E-01	25	D017	1 0 0 0 2	
4.577E-04	1.100E-01	25	D041	1 0 0 0 1	
4.661E-04	1.120E-01	25	L001	1 0 1 1 2	pH 6.0
4.910E-04	1.180E-01	27	D036	0 0 0 0 0	
7.100E-04	1.706E-01	34.99	C404	2 1 2 2 1	
8.500E-04	2.043E-01	44.99	C404	2 1 2 2 1	
2.163E-03	5.197E-01	75	D041	1 0 0 0 1	
4.536E-04	1.090E-01	rt	B103	0 0 0 0 2	

869. C₆H₁₂N₂O₄S

DL-Lanthionine

L-Cysteine, S-[(2R)-2-amino-2-carboxyethyl]-

RN: 922-55-4 MP (°C): 280

MW: 208.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.193E-03	1.498E+00	25	D041	1 0 0 0 1	

870. C₆H₁₂N₂O₄S₂

Mesocystine

meso-Cystine

RN: 6020-39-9 MP (°C):

MW: 240.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.330E-04	5.600E-02	25	L001	1 0 1 1 1	pH 6.0

871. C₆H₁₂N₂O₄S₂

D-Cystine

D-(+)-3,3'-Dithiobis(2-aminopropanoic acid)

RN: 349-46-2 MP (°C): 227

MW: 240.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.577E-04	1.100E-01	25	D041	1 0 0 0 1	
4.702E-04	1.130E-01	25	L001	1 0 1 1 2	pH 6.0

872. C₆H₁₂N₂O₄S₂

DL-Cystine

Cystine

RN: 923-32-0

MP (°C):

MW: 240.30

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.039E-04	4.900E-02	25	D041	1 0 0 0 1	
2.372E-04	5.700E-02	25	L001	1 0 1 1 1	pH 6.0

873. C₆H₁₂N₂S₄

Thiram

Tetramethylthioperoxydicarbonothioic diamine

Tetramethylthiuram disulfide

N,N'-(Dithiodicarbonothioyl)bis(N-methylmethanamine)

Arasan

Nomersan

RN: 137-26-8

MP (°C): 155.5

MW: 240.43

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.413E-05	1.782E-02	ns	R427	0 0 0 0 0	
1.248E-04	3.000E-02	rt	M161	0 0 0 0 1	

874. C₆H₁₂N₂S₄Zn

Ziram

Zinc bis dimethyldithiocarbamate

Corozate

Karbam white

Fuklasin

Fuclasin

RN: 137-30-4

MP (°C): 240

MW: 305.81

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.125E-04	6.500E-02	20	F300	1 0 0 0 1	
1.308E-05	4.000E-03	20	F311	1 2 2 2 1	<i>sic</i>
2.125E-04	6.500E-02	25	M161	1 0 0 0 1	

875. C₆H₁₂N₄

Methenamine

Hexamethylen-tetramin

RN: 100-97-0 **MP (°C):**
MW: 140.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.231E+00	3.128E+02	1.99	B442	0 0 0 0 0	
2.202E+00	3.087E+02	3.99	B442	0 0 0 0 0	
2.183E+00	3.060E+02	5.99	B442	0 0 0 0 0	
2.149E+00	3.012E+02	9.99	B442	0 0 0 0 0	
2.254E+00	3.161E+02	10.99	B442	0 0 0 0 0	
2.250E+00	3.154E+02	11.99	B442	0 0 0 0 0	
3.200E+00	4.486E+02	12	F300	1 0 0 0 2	
2.234E+00	3.131E+02	14.99	B442	0 0 0 0 0	
2.191E+00	3.072E+02	19.99	B442	0 0 0 0 0	
2.156E+00	3.023E+02	24.99	B442	0 0 0 0 0	
2.193E+00	3.074E+02	29.99	B442	0 0 0 0 0	
2.218E+00	3.110E+02	34.99	B442	0 0 0 0 0	
2.233E+00	3.131E+02	39.99	B442	0 0 0 0 0	

876. C₆H₁₂N₄O₂

2,6-Dimethyldinitrosopiperazine

DMDNP

RN: 55380-34-2 **MP (°C):**
MW: 172.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.066E+01	24	M031	1 1 1 1 1	

877. C₆H₁₂N₅O₂PS₂

Menazon

O,O-Dimethyl S-(4,6-diamino-1,3,5-triazinyl-2-methyl) dithiophosphate

RN: 78-57-9 **MP (°C):**
MW: 281.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.532E-04	2.400E-01	20	M161	1 0 0 0 1	
3.551E-03	9.990E-01	ns	M061	0 0 0 0 0	

878. C₆H₁₂O

Pinacolone

3,3-Dimethyl-2-butanone

3,3-Dimethylbutanone-2

RN: 75-97-8 **MP (°C):** -52.5
MW: 100.16 **BP (°C):** 106.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.376E-01	2.380E+01	15	F300	1 0 0 0 2	
1.996E-01	1.999E+01	20	G030	1 2 0 0 2	
1.862E-01	1.865E+01	25	G030	1 2 0 0 2	
1.817E-01	1.820E+01	25	K072	1 0 1 1 1	
1.736E-01	1.739E+01	30	G030	1 2 0 0 2	

879. C₆H₁₂O

Cyclohexanol

1-Cyclohexanol

Naxol

Cyclohexyl alcoho

Adrona

Hydrophenol

RN: 108-93-0 **MP (°C):** 23
MW: 100.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.357E-01	5.366E+01	11	F052	1 1 1 0 2	
5.391E-01	5.400E+01	11	F300	1 0 0 0 1	
1.296E-02	1.298E+00	20	D052	1 1 0 0 1	<i>sic</i>
3.283E-01	3.288E+01	25	B019	1 0 1 2 0	
3.283E-01	3.288E+01	25	B092	2 1 1 1 2	
3.469E-01	3.475E+01	25	C108	2 2 2 2 2	
3.800E-01	3.806E+01	25	F044	1 0 0 0 1	
3.766E-01	3.772E+01	25	H028	2 0 2 0 2	
3.655E-01	3.661E+01	35	C108	2 2 2 2 2	
3.264E-01	3.269E+01	60	B092	2 1 1 1 2	
3.766E-01	3.772E+01	ns	A406	0 0 0 0 1	

880. C₆H₁₂O

Isopropylacetone

4-Methyl-2-pentanone

Methyl isobutyl ketone

RN: 108-10-1 **MP (°C):** -80
MW: 100.16 **BP (°C):** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.070E-01	3.075E+01	0	G032	1 2 1 1 2	
2.310E-01	2.314E+01	10	G032	1 2 1 1 2	
1.871E-01	1.874E+01	20	D052	1 1 0 0 2	
1.996E-01	1.999E+01	20	G030	1 2 0 0 2	

(continued)

880. C₆H₁₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-01	1.961E+01	22.00	O005	2 0 2 2 0	
1.862E-01	1.865E+01	24.6	H121	2 0 0 0 1	
1.862E-01	1.865E+01	25	B060	2 0 1 1 1	
1.717E-01	1.720E+01	25	C329	1 1 1 1 1	average
1.871E-01	1.874E+01	25	G030	1 2 0 0 2	
2.340E-01	2.344E+01	25	K103	1 2 2 2 1	
1.862E-01	1.865E+01	25	L082	1 1 2 1 1	
1.736E-01	1.739E+01	25	L319	1 0 2 1 2	
1.817E-01	1.820E+01	25	M087	1 1 2 1 2	
1.669E-01	1.672E+01	25	R320	1 0 1 1 1	
1.746E-01	1.749E+01	30	G030	1 2 0 0 2	
1.660E-01	1.663E+01	30	G032	1 2 1 1 2	
1.410E-01	1.412E+01	50	G032	1 2 1 1 2	
4.720E+01	4.728E+03	53.0	R308	2 2 1 1 2	
1.669E-01	1.672E+01	70	L082	1 1 2 1 1	
1.370E-01	1.372E+01	75	G032	1 2 1 1 2	
4.300E+01	4.307E+03	97.0	R308	2 2 1 1 2	
4.088E+01	4.094E+03	108.0	R308	2 2 1 1 2	
3.902E+01	3.909E+03	120.0	R308	2 2 1 1 2	
3.333E-01	3.339E+01	125.0	R308	2 2 1 1 1	
5.278E-01	5.286E+01	151.0	R308	2 2 1 1 1	
3.425E+01	3.431E+03	153.0	R308	2 2 1 2 2	

881. C₆H₁₂O

2-Ethylbutanal

Ethyl butyraldehyde

2-Ethylbutyraldehyde

Diethyl acetaldehyde; ethyl butyraldehyde

Diethyl acetaldehyde

Ethyl butyraldehyde

RN: 97-96-1 MP (°C):

MW: 100.16 BP (°C): 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-02	3.025E+00	ns	S460	0 0 0 0 0	

882. C₆H₁₂O

Caproic aldehyde

Hexaldehyde

n-HexanalRN: 66-25-1 MP (°C):
MW: 100.16 BP (°C): 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.581E-01	5.590E+01	0	C423	0 0 0 0 0	
4.493E-01	4.500E+01	4	C423	0 0 0 0 0	

(continued)

882. C₆H₁₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.155E-01	3.160E+01	10	C423	0 0 0 0 0	
4.992E-02	5.000E+00	25	A049	1 0 1 0 1	
1.907E-01	1.910E+01	25	C435	0 0 0 0 0	
4.792E-02	4.800E+00	25	J418	0 0 0 0 0	

883. C₆H₁₂O

4-Methyl-3-pentanone

4-Methylpentanone-3

RN: 565-69-5 MP (°C):

MW: 100.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.601E-01	1.604E+01	20	G030	1 2 0 0 2	
1.495E-01	1.497E+01	25	G030	1 2 0 0 2	
1.398E-01	1.400E+01	30	G030	1 2 0 0 2	
1.549E-01	1.551E+01	ns	S460	0 0 0 0 0	

884. C₆H₁₂O

3-Methyl-2-pentanone

3-Methylpentanone-2

RN: 565-61-7 MP (°C): <25

MW: 100.16 BP (°C): 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.206E-01	2.210E+01	20	G030	1 2 0 0 2	
2.044E-01	2.047E+01	25	G030	1 2 0 0 2	
1.890E-01	1.893E+01	30	G030	1 2 0 0 2	

885. C₆H₁₂O

3-Hexanone

Hexanone-3

RN: 589-38-8 MP (°C): -55.5

MW: 100.16 BP (°C): 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-01	1.546E+01	20	G030	1 2 0 0 2	
1.446E-01	1.449E+01	25	G030	1 2 0 0 2	
1.359E-01	1.361E+01	30	G030	1 2 0 0 2	

886. C₆H₁₂O

2-Methyl-4-penten-3-ol

2-Methylpenten-4-ol-3

RN: 4798-45-2 **MP (°C):**
MW: 100.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-01	3.185E+01	20	G031	1 0 0 0 2	
2.964E-01	2.969E+01	25	G031	1 0 0 0 2	
2.804E-01	2.809E+01	30	G031	1 0 0 0 2	

887. C₆H₁₂O

1-Hexen-3-ol

Hexen-1-ol-3

RN: 4798-44-1 **MP (°C):**
MW: 100.16 **BP (°C):** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.644E-01	2.648E+01	20	G031	1 0 0 0 2	
2.454E-01	2.458E+01	25	G031	1 0 0 0 2	
2.302E-01	2.306E+01	30	G031	1 0 0 0 2	

888. C₆H₁₂O

Methyl butyl ketone

2-Hexanone

Methyl *n*-butyl ketone

RN: 591-78-6 **MP (°C):** -57
MW: 100.16 **BP (°C):** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.323E-01	4.330E+01	0	C423	0 0 0 0 0	
3.335E-01	3.340E+01	4	C423	0 0 0 0 0	
2.386E-01	2.390E+01	10	C423	0 0 0 0 0	
2.040E-01	2.043E+01	10	G032	1 2 1 1 2	
2.192E-02	2.195E+00	20	D052	1 1 0 0 1	<i>sic</i>
1.717E-01	1.720E+01	20	G030	1 2 0 0 2	
1.617E-01	1.620E+01	25	C435	0 0 0 0 0	
1.611E-01	1.614E+01	25	G030	1 2 0 0 2	
1.997E-01	2.000E+01	25	J418	0 0 0 0 0	
3.320E-01	3.326E+01	25	P055	1 0 0 0 2	
1.505E-01	1.507E+01	30	G030	1 2 0 0 2	
1.450E-01	1.452E+01	30	G032	1 2 1 1 2	
1.475E-01	1.478E+01	38	J020	2 1 2 1 1	
1.240E-01	1.242E+01	50	G032	1 2 1 1 2	

889. C₆H₁₂O

4-Hexen-3-ol

Hexen-4-ol-3

RN: 4798-58-7 **MP (°C):**
MW: 100.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.895E-01	3.902E+01	20	G031	1 0 0 0 2	
3.664E-01	3.670E+01	25	G031	1 0 0 0 2	
3.451E-01	3.456E+01	30	G031	1 0 0 0 2	

890. C₆H₁₂O₂

3-Hydroxy-2,2-dimethyltetrahydrofuran

3-Furanol, tetrahydro-2,2-dimethyl-

2,2-Dimethyltetrahydrofuran-3-ol

RN: 101398-19-0 **MP (°C):**
MW: 116.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.826E-01	9.091E+01	rt	B066	0 2 0 0 1	

891. C₆H₁₂O₂

Diethylacetic acid

2-Ethylbutyric acid

2-Ethyl-butanoic acid

Ethylbutyric acid

RN: 88-09-5 **MP (°C):** -15
MW: 116.16 **BP (°C):** 194.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.147E-02	2.494E+00	25	O011	1 0 1 1 1	

892. C₆H₁₂O₂

n-Caproic acid

n-Capronsaure

RN: 142-62-1 **MP (°C):** -3.4
MW: 116.16 **BP (°C):** 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.438E-02	8.640E+00	0	B136	1 0 2 1 2	
7.610E-02	8.840E+00	15	F300	1 0 0 0 2	
8.333E-02	9.680E+00	20	B136	1 0 2 1 2	
8.270E-02	9.607E+00	20	D041	1 0 0 0 1	
8.253E-02	9.587E+00	20	R001	1 1 1 1 2	
8.675E-02	1.008E+01	25	H028	2 0 2 0 2	

(continued)

892. C₆H₁₂O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.760E-02	1.018E+01	25	H122	1 0 0 0 2	
8.608E-02	9.999E+00	25	H339	2 2 1 2 2	
9.367E-02	1.088E+01	25	O011	1 0 1 1 1	
8.772E-02	1.019E+01	30	B136	1 0 2 1 2	
8.684E-02	1.009E+01	30	R001	1 1 1 1 2	
9.282E-02	1.078E+01	35	H339	2 2 1 2 2	
9.427E-02	1.095E+01	45	B136	1 0 2 1 2	
9.324E-02	1.083E+01	45	R001	1 1 1 1 2	
1.008E-01	1.171E+01	60	B136	1 0 2 1 2	
9.956E-02	1.156E+01	60	D041	1 0 0 0 2	
9.964E-02	1.157E+01	60	R001	1 1 1 1 2	
7.374E-02	8.566E+00	.0	R001	1 1 1 1 2	
8.692E-02	1.010E+01	ns	A406	0 0 0 0 1	

893. C₆H₁₂O₂*n*-Butyl acetateEssigsaeure-*n*-butyl ester*n*-Butylacetat

Butyl acetate

1-Butyl acetate

RN: 123-86-4

MP (°C): -90

MW: 116.16

BP (°C): 117.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.686E-02	4.282E+00	20	D052	1 1 0 0 0	
8.609E-02	1.000E+01	22	F300	1 0 0 0 0	
5.814E-02	6.754E+00	25	B060	2 0 1 1 1	
7.171E-02	8.330E+00	25	L319	1 0 2 1 2	
1.935E-01	2.248E+01	25	P055	1 0 0 0 1	
2.489E-02	2.892E+00	30	N330	2 2 2 1 2	
7.679E-02	8.920E+00	30	R318	1 1 0 1 0	
5.020E-02	5.831E+00	37	E028	1 0 1 1 2	
5.899E-02	6.853E+00	50	O012	1 2 1 1 2	

894. C₆H₁₂O₂

Pentyl formate

n-Amyl formate

RN: 638-49-3

MP (°C):

MW: 116.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	2.904E+00	22	S006	1 0 0 0 1	

895. C₆H₁₂O₂

Ethyl butyrate

Butanoic acid ethyl ester

Ethyl butanoate

Butyric ether

RN: 105-54-4**MP (°C):** -135.4**MW:** 116.16**BP (°C):** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.410E-02	2.800E+00	0	C423	0 0 0 0 0	
2.763E-02	3.210E+00	4	C423	0 0 0 0 0	
3.151E-02	3.660E+00	10	C423	0 0 0 0 0	
4.198E-02	4.876E+00	20	D052	1 1 0 0 1	
5.310E-02	6.168E+00	22	F001	1 0 1 2 2	
4.300E-02	4.995E+00	22	S006	1 0 0 0 1	
3.702E-02	4.300E+00	25	C435	0 0 0 0 0	
6.832E-02	7.937E+00	30	R318	1 1 0 1 0	

896. C₆H₁₂O₂*sec*-Butyl acetateDL-*sec*-Butyl acetate**RN:** 105-46-4**MP (°C):****MW:** 116.16**BP (°C):** 114

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.305E-02	6.162E+00	20	D052	1 1 0 0 0	

897. C₆H₁₂O₂

3-Hydroxy-2,5-dimethyltetrahydrofuran

3-Furanol, tetrahydro-2,5-dimethyl-

RN: 30003-26-0 **MP (°C):****MW:** 116.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.435E+00	1.667E+02	rt	B066	0 2 0 0 1	

898. C₆H₁₂O₂

Propyl propionate

Propionic acid *N*-propyl ester*n*-Propyl propionate**RN:** 106-36-5**MP (°C):****MW:** 116.16**BP (°C):** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	5.808E+00	22	S006	1 0 0 0 0	

899. C₆H₁₂O₂

Isobutyl acetate

Acetic acid isobutyl ester

Essigsaeureisobutyl ester

RN: 110-19-0 **MP (°C):** -99
MW: 116.16 **BP (°C):** 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.502E-02	7.553E+00	14.60	L310	2 2 1 1 2	
5.729E-02	6.655E+00	20	D052	1 1 0 0 1	
5.800E-02	6.737E+00	20	F001	1 0 1 2 1	
5.768E-02	6.700E+00	20	F300	1 0 0 0 1	
6.154E-02	7.149E+00	24.90	L310	2 2 1 1 2	
5.390E-02	6.261E+00	25	B060	2 0 1 1 1	
5.967E-02	6.932E+00	47.90	L310	2 2 1 1 2	
6.154E-02	7.149E+00	67.60	L310	2 2 1 1 2	
6.493E-02	7.543E+00	74.90	L310	2 2 1 1 2	
6.502E-02	7.553E+00	75.20	L310	2 2 1 1 2	
6.875E-02	7.986E+00	84.80	L310	2 2 1 1 2	
7.205E-02	8.369E+00	93.20	L310	2 2 1 1 2	
8.253E-02	9.587E+00	111.50	L310	2 2 1 1 2	
8.540E-02	9.921E+00	115.70	L310	2 2 1 1 2	
1.026E-01	1.192E+01	147.10	L310	2 2 1 1 2	

900. C₆H₁₂O₃

Paraldehyde

Paraldehyd

RN: 123-63-7 **MP (°C):** 12.6
MW: 132.16 **BP (°C):** 128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.853E-01	1.170E+02	8.5	P059	1 1 1 0 1	
8.377E-01	1.107E+02	11.5	P059	1 1 1 0 1	
8.287E-01	1.095E+02	12.0	P059	1 1 1 0 1	
8.323E-01	1.100E+02	13	F300	1 0 0 0 1	
8.047E-01	1.063E+02	13.5	P059	1 1 1 0 1	
7.621E-01	1.007E+02	17.0	P059	1 1 1 0 1	
6.311E-01	8.341E+01	27.0	P059	1 1 1 0 1	
8.475E-01	1.120E+02	30	F300	1 0 0 0 2	
5.377E-01	7.106E+01	40.0	P059	1 1 1 0 1	
5.246E-01	6.933E+01	42.5	P059	1 1 1 0 1	
4.283E-01	5.660E+01	68.0	P059	1 1 1 0 1	
4.148E-01	5.482E+01	75.0	P059	1 1 1 0 1	
4.540E-01	6.000E+01	100	F300	1 0 0 0 0	

901. C₆H₁₂O₃

2-Ethoxyethyl acetate

Cellosolve acetate

RN: 111-15-9 **MP (°C):** -61
MW: 132.16 **BP (°C):** 156

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.499E+00	1.981E+02	20	D052	1 1 0 0 2	
1.415E+00	1.870E+02	20	M062	1 0 0 0 2	

902. C₆H₁₂O₃

Methyl β-ethoxypropionate

Methyl 3-ethoxypropionate

3-Ethoxypropionic acid methyl ester

RN: 14144-33-3 **MP (°C):**
MW: 132.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.621E-01	1.007E+02	25	D002	1 2 1 1 2	
7.621E-01	1.007E+02	25	R034	0 0 0 0 2	

903. C₆H₁₂O₅

D-Quercitol

D-Quercit

RN: 488-73-3 **MP (°C):** 234
MW: 164.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.701E-01	1.100E+02	20	F300	1 0 0 0 2	

904. C₆H₁₂O₅

Rhamnose

α-L-Rhamnose

6-Deoxy-L-mannose

L-Mannomethylose

L-Rhamnose

RN: 3615-41-6 **MP (°C):** 82
MW: 164.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.212E+00	3.631E+02	18	D041	1 0 0 0 1	
3.177E+00	5.215E+02	40	D041	1 0 0 0 1	

905. C₆H₁₂O₆

D-Inositol

D(+)-Inositol

D-Chiro-inositol

(+) -Chiro-inositol

RN: 643-12-9

MP (°C): 249.5

MW: 180.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E+00	4.034E+02	11	F300	1 0 0 0 2	

906. C₆H₁₂O₆

D-Mannose

D-(+)-Mannose

Seminose

Carubinose

RN: 3458-28-4

MP (°C): 132

MW: 180.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.956E+00	7.126E+02	17	D041	1 0 0 0 2	
3.957E+00	7.128E+02	17	F300	1 0 0 0 2	
2.399E+00	4.322E+02	25	G317	0 0 0 0 0	

907. C₆H₁₂O₆

Glucose

D-Glucose

D(+)-Glucose

Staleydex 111

Staleydex 333

RN: 50-99-7

MP (°C): 146

MW: 180.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.954E+00	3.520E+02	.50	J019	1 0 1 2 2	
1.749E+00	3.151E+02	0	M043	1 0 0 0 1	
2.286E+00	4.118E+02	10	M043	1 0 0 0 1	
2.271E+00	4.091E+02	10.0	Y020	1 1 2 1 2	
3.365E+00	6.063E+02	15	D041	1 0 0 0 2	
2.660E+00	4.792E+02	20	M043	1 0 0 0 1	
2.314E+00	4.168E+02	20.0	Y020	1 1 2 1 2	
3.033E+00	5.464E+02	30	J019	1 0 1 2 2	
3.031E+00	5.460E+02	30	K122	1 1 1 1 2	
3.028E+00	5.455E+02	30	M043	1 0 0 0 2	
2.355E+00	4.244E+02	30.0	Y020	1 1 2 1 2	
1.901E+00	3.425E+02	30.50	M137	2 1 2 2 2	
2.042E+00	3.678E+02	35	B354	0 0 0 0 0	

(continued)

907. C₆H₁₂O₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.416E+00	6.154E+02	40	M043	1 0 0 0 2	
2.396E+00	4.317E+02	40.0	Y020	1 1 2 1 2	
3.936E+00	7.091E+02	50	J019	1 0 1 2 2	
2.436E+00	4.388E+02	50.0	Y020	1 1 2 1 2	
4.090E+00	7.368E+02	60	M043	1 0 0 0 2	
4.005E+00	7.215E+02	70	A420	0 0 0 0 0	
4.523E+00	8.148E+02	80	M043	1 0 0 0 2	
2.227E+00	4.012E+02	.0	Y020	1 1 2 1 2	
2.501E+00	4.505E+02	rt	D021	0 0 1 1 2	

908. C₆H₁₂O₆

Fructose

D-Fructose

D-(–)-Fructose

D-(–)-Levulose

Krystar 300

Nevulose

RN: 57-48-7

MP (°C): 129

MW: 180.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.379E+00	4.286E+02	0	M043	1 0 0 0 1	
4.318E+00	7.780E+02	20	F300	1 0 0 0 2	
2.467E+00	4.444E+02	20	M043	1 0 0 0 1	
4.524E+00	8.150E+02	30	K122	1 1 1 1 2	
4.524E+00	8.150E+02	30	K135	1 1 1 1 2	
2.448E+01	4.410E+03	30	K136	1 1 1 1 2	
2.550E+00	4.595E+02	40	M043	1 0 0 0 1	
2.629E+00	4.737E+02	60	M043	1 0 0 0 1	
4.709E+00	8.484E+02	70	A420	0 0 0 0 0	

909. C₆H₁₂O₆

Tagatose

Lyxo-2-hexulose

DL-Tagatose

RN: 17598-81-1

MP (°C):

MW: 180.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.084E+00	3.755E+02	22	F300	1 0 0 0 2	

910. C₆H₁₂O₆

D-Galactose

Galactose

(+) -Galactose

D(+) -Galactose

RN: 59-23-4**MP (°C):** 169**MW:** 180.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.046E-01	9.091E+01	0	D041	1 0 0 0 1	
2.247E+00	4.048E+02	25	D041	1 0 0 0 1	
2.253E+00	4.058E+02	rt	D021	0 0 1 1 2	

911. C₆H₁₂O₆

L-Sorbose

Sorbose

L-1,3,4,5,6-Pentahydroxyhexan-2-one

L-Xylo-2-hexulose

RN: 87-79-6**MP (°C):** 165**MW:** 180.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.970E+00	3.548E+02	17	D041	1 0 0 0 1	
1.998E+00	3.600E+02	17	F300	1 0 0 0 1	

912. C₆H₁₂O₆

Inositol

Mesoinositol

cis-1,2,3,5-trans-4,6-Cyclohexanehexol

Dambrose

Nucite

Phaseomannite

RN: 87-89-8**MP (°C):** 226**MW:** 180.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.788E-01	1.403E+02	19	F300	1 0 0 0 2	
8.267E-01	1.489E+02	20	D041	1 0 0 0 2	
7.771E-01	1.400E+02	25	M054	1 0 0 0 1	
7.771E-01	1.400E+02	ns	L335	0 0 0 0 2	
7.762E-01	1.398E+02	ns	R424	0 0 0 0 0	

913. C₆H₁₂O₆

α-Glucose

α-D-Glucose

D-α-Glucose

Dextrose

RN: 492-62-6**MP (°C):** 154.5**MW:** 180.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.355E+00	2.441E+02	0	D041	1 0 0 0 2	
2.019E+00	3.638E+02	10.0	Y020	1 1 2 1 2	
2.775E+00	5.000E+02	20	F300	1 0 0 0 0	
2.096E+00	3.775E+02	20.0	Y020	1 1 2 1 2	
2.501E+00	4.505E+02	25	D041	1 0 0 0 2	
2.170E+00	3.909E+02	30.0	Y020	1 1 2 1 2	
2.242E+00	4.040E+02	40.0	Y020	1 1 2 1 2	
2.313E+00	4.168E+02	50.0	Y020	1 1 2 1 2	
2.346E+00	4.227E+02	54.7	Y020	1 1 2 1 2	
1.942E+00	3.498E+02	.0	Y020	1 1 2 1 2	

914. C₆H₁₂O₆H₂O

Glucose (monohydrate)

RN: 50-99-7**MP (°C):** 83**MW:** 198.17**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E+00	2.871E+02	10.0	Y020	1 1 2 1 2	
1.619E+00	3.209E+02	20.0	Y020	1 1 2 1 2	
1.781E+00	3.530E+02	30.0	Y020	1 1 2 1 2	
1.933E+00	3.831E+02	40.0	Y020	1 1 2 1 2	
2.072E+00	4.106E+02	50.0	Y020	1 1 2 1 2	
1.784E+00	3.536E+02	73.2	Y020	1 1 2 1 2	
1.274E+00	2.525E+02	.0	Y020	1 1 2 1 2	

915. C₆H₁₂O₇

Scyllitol

Scyllit

Quercinitol

Cocositol

RN: 488-59-5**MP (°C):** 253**MW:** 196.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.149E-02	1.010E+01	18	F300	1 0 0 0 2	

916. C₆H₁₃Br

1-Bromohexane

Hexyl bromide

RN: 111-25-1 **MP (°C):** -84.7
MW: 165.08 **BP (°C):** 155.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-04	2.575E-02	25	M342	1 0 1 1 2	

917. C₆H₁₃N

1-Methylpiperidine

N-Methylpiperidine

RN: 626-67-5 **MP (°C):** -18
MW: 99.18 **BP (°C):** 106

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
+1.70E+00	+1.68E+02	ns	S460	0 0 0 0 0	

918. C₆H₁₃NO

Caproamide

n-Capronsaure-amid

Hexanamide

Hexanoic acid, amide

RN: 628-02-4 **MP (°C):** 99
MW: 115.18 **BP (°C):** 255

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-01	1.854E+01	6	H059	0 0 0 0 0	
2.030E-01	2.338E+01	16	H059	0 0 0 0 0	
2.580E-01	2.972E+01	25	H059	0 0 0 0 0	
2.750E-01	3.167E+01	29	H059	0 0 0 0 0	
3.150E-01	3.628E+01	33	H059	0 0 0 0 0	
3.250E-01	3.743E+01	35	H059	0 0 0 0 0	
3.390E-01	3.904E+01	37	H059	0 0 0 0 0	
3.890E-01	4.480E+01	41	H059	0 0 0 0 0	

919. C₆H₁₃NO₂

L-Norleucine

Norleucine

α-Aminocaproic acid

RN: 327-57-1 **MP (°C):** 327dec
MW: 131.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.304E-01	1.710E+01	23	K060	1 2 0 0 2	
1.127E-01	1.478E+01	25	D041	1 0 0 0 1	
8.700E-02	1.141E+01	25	E015	1 2 1 1 1	
1.232E-01	1.616E+01	25	K031	2 1 2 1 2	

920. C₆H₁₃NO₂

L-Leucine

L(-)-Leucine

Leucine

2-Amino-4-methylpentanoic acid

L-2-Amino-4-methylpentanoic acid

(2S)-α-Leucine

RN: 61-90-5**MP (°C):** 286–288**MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.692E-01	2.220E+01	0	F300	1 0 0 0 2	
1.740E-01	2.282E+01	15	D349	2 1 1 2 2	
1.601E-01	2.100E+01	20	B032	1 2 2 1 2	
1.800E-01	2.361E+01	20	D349	2 1 1 2 2	
1.695E-01	2.224E+01	21	P045	1 0 2 1 2	
1.772E-01	2.324E+01	24.99	C404	2 1 2 2 1	
1.640E-01	2.151E+01	25	B032	1 2 2 1 2	
1.712E-01	2.246E+01	25	C018	0 0 0 0 0	
1.851E-01	2.428E+01	25	C018	0 0 0 0 0	
1.700E-04	2.230E-02	25	C405	2 1 2 2 2	intrinsic zwit
1.883E-01	2.470E+01	25	D016	1 0 0 0 2	
1.634E-01	2.143E+01	25	D041	1 0 0 0 2	
1.860E-01	2.440E+01	25	D349	2 1 1 2 2	
1.807E-01	2.370E+01	25	F300	1 0 0 0 2	
1.626E-01	2.133E+01	25	G092	2 1 1 1 1	
1.626E-01	2.133E+01	25	G315	0 0 0 0 0	
1.647E-01	2.160E+01	25.1	N024	0 0 0 0 0	
1.654E-01	2.170E+01	25.1	N025	0 0 0 0 0	
1.647E-01	2.160E+01	25.1	N026	0 0 0 0 0	
1.612E-01	2.114E+01	25.1	N027	1 1 2 2 2	
1.765E-01	2.315E+01	27	D036	0 0 0 0 0	
1.601E-01	2.100E+01	27	D036	0 0 0 0 0	
1.682E-01	2.206E+01	29.80	B032	1 2 2 1 2	
1.907E-01	2.502E+01	34.99	C404	2 1 2 2 1	
2.041E-01	2.677E+01	44.99	C404	2 1 2 2 1	
2.142E-01	2.810E+01	50	F300	1 0 0 0 2	
2.805E-01	3.679E+01	75	D041	1 0 0 0 2	
2.805E-01	3.680E+01	75	F300	1 0 0 0 2	
2.886E-01	3.786E+01	92	M160	2 1 1 1 0	
4.071E-01	5.340E+01	100	F300	1 0 0 0 2	
4.069E-01	5.337E+01	99.99	P349	0 0 0 0 0	
1.830E-01	2.400E+01	ns	D072	0 0 0 0 1	

921. C₆H₁₃NO₂L-*allo*-Isoleucine

Alloisoleucine

RN: 1509-34-8**MP (°C):** >280**MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.148E-01	2.818E+01	20	D041	1 0 0 0 1	

922. C₆H₁₃NO₂

D-Leucine

D-2-Amino-4-methylvaleric acid

D-2-Amino-4-methylpentanoic acid

RN: 328-38-1 **MP (°C):** >300**MW:** 131.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-01	2.153E+01	25	D041	1 0 0 0 2	
1.975E-01	2.591E+01	50	D041	1 0 0 0 2	

923. C₆H₁₃NO₂

D-Norleucine

D-2-Amino-*n*-caproic acid

D-2-Aminohexanoic acid

RN: 327-56-0 **MP (°C):** >300**MW:** 131.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.201E-01	1.575E+01	19	D041	1 0 0 0 1	

924. C₆H₁₃NO₂*tert*-Amyl carbamate*tert*-Pentyl carbamate**RN:** 590-60-3 **MP (°C):** 85**MW:** 131.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-01	2.099E+01	37	H006	1 2 2 1 1	

925. C₆H₁₃NO₂*n*-Amyl carbamate*n*-Pentyl carbamate*O*-Pentyl carbamate**RN:** 638-42-6 **MP (°C):****MW:** 131.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	4.460E+00	37	H006	1 2 2 1 1	

926. C₆H₁₃NO₂

Isopentyl urethane

Isoamylurethan

Isoamylurethane

RN: 543-86-2**MP (°C):****MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.660E-02	4.801E+00	15.5	F001	1 0 1 2 2	

927. C₆H₁₃NO₂

ε-Aminocaproic acid

6-Aminocaproic acid

ε-Amino-capronsaeure

RN: 60-32-2**MP (°C):** 205**MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.848E+00	5.048E+02	25	M024	1 2 0 1 2	

928. C₆H₁₃NO₂

DL-Norleucine

DL-2-Amino-*n*-caproic acid

2-Aminohexanoic acid

DL-2-Aminohexanoic acid

RN: 616-06-8**MP (°C):** >300**MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.863E-02	9.003E+00	0	D018	2 2 2 1 2	
8.660E-02	1.136E+01	25	C018	0 0 0 0 0	
8.767E-02	1.150E+01	25	D016	1 0 0 0 2	
8.906E-02	1.168E+01	25	D018	2 2 2 1 2	
8.891E-02	1.166E+01	25	D041	1 0 0 0 2	
8.118E-02	1.065E+01	25	K031	2 1 2 1 2	
8.660E-02	1.136E+01	25	M024	1 2 0 1 2	
1.348E-01	1.768E+01	50	D018	2 2 2 1 2	
2.135E-01	2.800E+01	75	D018	2 2 2 1 2	
2.134E-01	2.799E+01	75	D041	1 0 0 0 2	
3.788E-01	4.969E+01	99.99	P349	0 0 0 0 0	

929. C₆H₁₃NO₂

L-Isoleucine

L(+)-Isoleucin

Isoleucine

RN: 73-32-5**MP (°C):** 288**MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.844E-01	3.730E+01	15.50	F300	1 0 0 0 2	
2.533E-01	3.323E+01	20	B032	1 2 2 1 2	
2.619E-01	3.435E+01	25	B032	1 2 2 1 2	
3.017E-01	3.957E+01	25	D041	1 0 0 0 2	
2.458E-01	3.224E+01	25	G433	0 0 0 0 0	
2.364E-01	3.101E+01	25	O316	1 0 1 2 2	
2.358E-01	3.093E+01	25	O316	1 0 1 2 2	
2.714E-01	3.560E+01	27	D036	0 0 0 0 0	
2.690E-01	3.528E+01	29.80	B032	1 2 2 1 2	
4.369E-01	5.732E+01	75	D041	1 0 0 0 2	
3.801E-01	4.985E+01	84	M160	2 1 1 1 0	

930. C₆H₁₃NO₂

α-Hydroxycaproamide

Hexanamide, 2-hydroxy-

2-Hydroxyhexanamide

RN: 66461-73-2**MP (°C):****MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.300E-02	1.089E+01	25	M008	1 0 0 0 2	

931. C₆H₁₃NO₂

N-Propylurethane

Propylurethan

n-Propyl urethane

RN: 623-85-8**MP (°C):****MW:** 131.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.475E-01	9.805E+01	15.5	F001	1 0 1 2 2	

932. C₆H₁₃NO₂

DL-Isoleucine

DL-2-Amino-3-methylpentanoic acid

RN: 443-79-8 MP (°C):

MW: 131.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-01	1.720E+01	0	D018	2 2 2 1 2	
1.632E-01	2.141E+01	25	D018	2 2 2 1 2	
1.662E-01	2.180E+01	25	D041	1 0 0 0 2	
2.235E-01	2.931E+01	50	D018	2 2 2 1 2	
3.510E-01	4.605E+01	75	D018	2 2 2 1 2	
3.357E-01	4.404E+01	75	D041	1 0 0 0 2	
5.517E-01	7.237E+01	99.99	P349	0 0 0 0 0	

933. C₆H₁₃NO₂

DL-Leucine

DL-2-Amino-4-methylvaleric acid

DL-2-Amino-4-methylpentanoic acid

RN: 328-39-2 MP (°C): 295

MW: 131.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.659E-02	8.735E+00	0	D018	2 2 2 1 2	
6.022E-02	7.900E+00	0	F300	1 0 0 0 1	
7.433E-02	9.750E+00	25	C018	0 0 0 0 0	
7.517E-02	9.860E+00	25	D016	1 0 0 0 2	
8.898E-02	1.167E+01	25	D018	2 2 2 1 2	
7.481E-02	9.813E+00	25	D041	1 0 0 0 2	
7.471E-02	9.800E+00	25	F300	1 0 0 0 1	
1.321E-01	1.733E+01	50	D018	2 2 2 1 2	
1.060E-01	1.390E+01	50	F300	1 0 0 0 2	
2.105E-01	2.762E+01	75	D018	2 2 2 1 2	
1.696E-01	2.225E+01	75	D041	1 0 0 0 2	
1.700E-01	2.230E+01	75	F300	1 0 0 0 2	
3.080E-01	4.040E+01	100	F300	1 0 0 0 2	
3.077E-01	4.036E+01	99.99	P349	0 0 0 0 0	
7.324E-02	9.607E+00	rt	H431	0 0 0 0 0	average

934. C₆H₁₄

Hexane

Normal hexane

n-Hexane

Skellysolve B

RN: 110-54-3 MP (°C): -95

MW: 86.18 BP (°C): 65

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.915E-04	1.650E-02	0	P003	2 2 2 2 2	
1.900E-04	1.637E-02	4.0	N004	1 1 2 2 2	

(continued)

934. C₆H₁₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.761E-04	1.518E-02	14.0	N004	1 1 2 2 2	
1.600E-03	1.379E-01	15.5	F001	1 0 1 0 2	
6.382E-04	5.500E-02	16	D047	1 0 0 1 1	
1.427E-04	1.230E-02	25	A058	1 1 1 1 2	
1.624E-03	1.400E-01	25	A094	1 0 0 0 1	
1.625E-03	1.400E-01	25	K072	1 0 1 1 1	
1.857E-03	1.600E-01	25	K112	1 0 2 1 1	
1.860E-03	1.603E-01	25	K112	1 0 2 2 2	
1.099E-04	9.470E-03	25	K119	1 0 0 0 2	
1.427E-04	1.230E-02	25	L002	2 2 2 2 2	
1.102E-04	9.500E-03	25	M001	2 1 2 2 2	
1.102E-04	9.500E-03	25	M002	2 1 2 2 2	
1.102E-04	9.500E-03	25	M040	1 0 0 1 1	
1.625E-03v	1.400E-01	25	M087	1 1 2 1 1	
1.430E-04	1.232E-02	25	M342	1 0 1 1 2	
1.439E-04	1.240E-02	25	P003	2 2 2 2 2	
1.624E-03	1.400E-01	25	S012	2 0 2 2 1	
2.128E-04	1.834E-02	25.0	N004	1 1 2 2 2	
1.099E-04	9.470E-03	25.0	P051	2 1 1 2 2	
1.099E-04	9.470E-03	25.00	P007	2 1 2 2 2	
1.494E-04	1.288E-02	35.0	N004	1 1 2 2 2	
4.623E-02	3.984E+00	38	J020	2 0 2 1 0	sic
1.172E-04	1.010E-02	40.1	P051	2 1 1 2 2	
1.172E-04	1.010E-02	40.10	P007	2 1 2 2 2	
2.578E-04	2.221E-02	45.0	N004	1 1 2 2 2	
2.553E-03	2.200E-01	50	L097	1 1 1 1 1	
2.456E-04	2.116E-02	55.0	N004	1 1 2 2 2	
1.532E-04	1.320E-02	55.7	P051	2 1 1 2 2	
1.532E-04	1.320E-02	55.70	P007	2 1 2 2 2	
1.775E-04	1.530E-02	69.7	P051	2 1 1 2 2	average of 2
1.764E-04	1.520E-02	69.70	P007	2 1 2 2 2	
1.787E-04	1.540E-02	69.70	P007	2 1 2 2 2	
2.599E-04	2.240E-02	99.1	P051	2 1 1 2 2	
2.599E-04	2.240E-02	99.10	P007	2 1 2 2 2	
3.388E-04	2.920E-02	114.4	P051	2 1 1 2 2	
3.388E-04	2.920E-02	114.40	P007	2 1 2 2 2	
4.363E-04	3.760E-02	121.3	P051	2 1 1 2 2	
4.363E-04	3.760E-02	121.30	P007	2 1 2 2 2	
6.603E-04	5.690E-02	137.3	P051	2 1 1 2 2	
6.603E-04	5.690E-02	137.30	P007	2 1 2 2 2	
1.230E-03	1.060E-01	151.8	P051	2 1 1 2 2	
1.230E-03	1.060E-01	151.80	P007	2 1 2 2 2	
1.102E-04	9.500E-03	ns	H123	0 0 0 0 0	
1.392E-03	1.200E-01	ns	M010	0 0 0 0 1	
1.880E-04	1.620E-02	ns	M175	0 0 2 1 2	

935. C₆H₁₄

2,2-Dimethylbutane

Neohexane

RN: 75-83-2

MP (°C): -100

MW: 86.18

BP (°C): 50

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.572E-04	3.940E-02	0	P003	2 2 2 2 2	
4.278E-04	3.686E-02	2.34	S461	0 0 0 0 0	
3.444E-04	2.968E-02	9.99	S461	0 0 0 0 0	
2.722E-04	2.346E-02	24.99	S461	0 0 0 0 0	
2.460E-04	2.120E-02	25	K119	1 0 0 0 2	
2.135E-04	1.840E-02	25	M001	2 1 2 2 2	
2.135E-04	1.840E-02	25	M002	2 1 2 2 2	
2.762E-04	2.380E-02	25	P003	2 2 2 2 2	
2.460E-04	2.120E-02	25	P051	2 1 1 2 2	
2.460E-04	2.120E-02	25.00	P007	2 1 2 2 2	
6.600E-04	5.687E-02	ns	J300	0 0 0 0 0	

936. C₆H₁₄

2,3-Dimethylbutane

Diisopropyl

1,1,2,2-Tetramethylethane

RN: 79-29-8

MP (°C): -129

MW: 86.18

BP (°C): 58

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.818E-04	3.290E-02	0	P003	2 2 2 2 2	
2.216E-04	1.910E-02	25	K119	1 0 0 0 2	
2.611E-04	2.250E-02	25	P003	2 2 2 2 2	
2.216E-04	1.910E-02	25.0	P051	2 1 1 2 2	
2.216E-04	1.910E-02	25.00	P007	2 1 2 2 2	
2.228E-04	1.920E-02	40.1	P051	2 1 1 2 2	
2.228E-04	1.920E-02	40.10	P007	2 1 2 2 2	
2.750E-04	2.370E-02	55.1	P051	2 1 1 2 2	
2.750E-04	2.370E-02	55.10	P007	2 1 2 2 2	
4.653E-04	4.010E-02	99.1	P051	2 1 1 2 2	
4.653E-04	4.010E-02	99.10	P007	2 1 2 2 2	
6.591E-04	5.680E-02	121.3	P051	2 1 1 2 2	
6.591E-04	5.680E-02	121.30	P007	2 1 2 2 2	
1.136E-03	9.790E-02	137.3	P051	2 1 1 2 2	
1.136E-03	9.790E-02	137.30	P007	2 1 2 2 2	
1.984E-03	1.710E-01	149.5	P051	2 1 1 2 2	
1.984E-03	1.710E-01	149.50	P007	2 1 2 2 2	

937. C₆H₁₄

2-Methylpentane

2-Metylpentan

RN: 107-83-5**MP (°C):** -154**MW:** 86.18**BP (°C):** 62

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.257E-04	1.945E-02	0	P003	2 2 2 2 2	
5.976E-04	5.150E-02	23	C332	0 0 0 0 0	
1.508E-04	1.300E-02	25	K119	1 0 0 0 2	
1.648E-04	1.420E-02	25	L002	2 2 2 2 2	
1.601E-04	1.380E-02	25	M001	2 1 2 2 2	
1.601E-04	1.380E-02	25	M002	2 1 2 2 2	
1.822E-04	1.570E-02	25	P003	2 2 2 2 2	
1.508E-04	1.300E-02	25.0	P051	2 1 1 2 2	
1.508E-04	1.300E-02	25.00	P007	2 1 2 2 2	
1.601E-04	1.380E-02	40.1	P051	2 1 1 2 2	
1.601E-04	1.380E-02	40.10	P007	2 1 2 2 2	
1.822E-04	1.570E-02	55.7	P051	2 1 1 2 2	
1.822E-04	1.570E-02	55.70	P007	2 1 2 2 2	
3.145E-04	2.710E-02	99.1	P051	2 1 1 2 2	
3.145E-04	2.710E-02	99.10	P007	2 1 2 2 2	
5.210E-04	4.490E-02	118.0	P051	2 1 1 2 2	
5.210E-04	4.490E-02	118.00	P007	2 1 2 2 2	
1.007E-03	8.680E-02	137.3	P051	2 1 1 2 2	
1.007E-03	8.680E-02	137.30	P007	2 1 2 2 2	
1.311E-03	1.130E-01	149.50	P007	2 1 2 2 2	

938. C₆H₁₄

3-Methylpentane

3-Metylpentan

RN: 96-14-0**MP (°C):** -118**MW:** 86.18**BP (°C):** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.495E-04	2.150E-02	0	P003	2 2 2 2 2	
1.520E-04	1.310E-02	25	K119	1 0 0 0 2	
1.485E-04	1.280E-02	25	M001	2 1 2 2 2	
2.077E-04	1.790E-02	25	P003	2 2 2 2 2	
1.520E-04	1.310E-02	25	P051	2 1 1 2 2	
1.520E-04	1.310E-02	25.00	P007	2 1 2 2 2	
1.485E-04	1.280E-02	ns	H123	0 0 0 0 0	

939. C₆H₁₄FO₃P

Isofluorophate

Diisopropylfluorophosphate

Phosphorofluoridic acid bis(1-methylethyl) ester

Difluorophate

PF-3

T-1703

RN: 55-91-4 **MP (°C):** -82**MW:** 184.15 **BP (°C):** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.236E-02	1.517E+01	25	D041	1 0 0 0 2	

940. C₆H₁₄NO₃PS₂

Ethoate-methyl

O,O-Dimethyl S-(N-ethylcarbamoylmethyl) dithiophosphate

Fitios

RN: 116-01-8 **MP (°C):** 66.1**MW:** 243.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.494E-02	8.500E+00	25	M061	1 0 0 0 1	
3.494E-02	8.500E+00	25	M161	1 0 0 0 1	

941. C₆H₁₄N₂

trans-2,5-Dimethylpiperazine

trans-2,5-Dimethyl-piperazin

RN: 2815-34-1 **MP (°C):****MW:** 114.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.065E+00	3.500E+02	20	F300	1 0 0 0 1	

942. C₆H₁₄N₂OMethyl-*n*-amylnitrosamine*N*-Nitroso(methyl)pentylamine**RN:** 13256-07-0 **MP (°C):****MW:** 130.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-02	1.094E+01	24	D083	2 0 0 0 1	

943. C₆H₁₄N₂ODi-*n*-propylnitrosamine*N*-Nitroso-*N*-propyl-1-propanamine

Dipropylnitrosamine

NDPA

DPNA

Nitrosodipropylamine

RN: 621-64-7 **MP (°C):****MW:** 130.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-02	9.895E+00	24	D083	2 0 0 0 1	

944. C₆H₁₄N₂OEthyl-*n*-butylnitrosamineNitroso-*N*-ethyl-*n*-butylamine*N*-Nitroso-*N*-butylethylamine*N*-Nitroso(ethyl)-*n*-butylamine

NEBA

Butanamine, *N*-ethyl-*N*-nitroso-**RN:** 4549-44-4 **MP (°C):****MW:** 130.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.200E-02	1.198E+01	24	D083	2 0 0 0 1	

945. C₆H₁₄N₂O

Di-isopropylnitrosamine

2-Propanamine, *N*-(1-methylethyl)-*N*-nitroso-*N*-Nitrosodiisopropylamine

NDiPA

RN: 601-77-4 **MP (°C):****MW:** 130.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.302E+01	24	D083	2 0 0 0 1	

946. C₆H₁₄N₂O₂

L(+)-Lysine

L(+)-Lysin

Lysine

RN: 56-87-1 **MP (°C):** 224**MW:** 146.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.995E+00	5.840E+02	27	D036	0 0 0 0 0	

947. C₆H₁₄N₄O₂

DL-Arginine

(±)-Arginine

RN: 7200-25-1**MP (°C):****MW:** 174.20**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.382E+00	2.407E+02	20	J303	0 0 0 0 0	
1.978E+00	3.445E+02	40	J303	0 0 0 0 0	
2.781E+00	4.844E+02	50	J303	0 0 0 0 0	
3.851E+00	6.709E+02	60	J303	0 0 0 0 0	

948. C₆H₁₄N₄O₂

L-Arginine

L(+)-Arginin

Arginine

RN: 74-79-3**MP (°C):** 244**MW:** 174.20**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.559E-01	1.143E+02	10	H062	1 2 2 0 0	EFG
8.588E-01	1.496E+02	20	B032	1 2 2 1 2	
7.487E-01	1.304E+02	21	D041	1 0 0 0 1	
8.037E-01	1.400E+02	21	F300	1 0 0 0 0	average
1.044E+00	1.818E+02	25	B032	1 2 2 1 2	
9.230E-01	1.608E+02	25	G315	0 0 0 0 0	
3.060E+00	5.330E+02	27	D036	0 0 0 0 0	
1.241E+00	2.162E+02	29.80	B032	1 2 2 1 2	
1.111E+00	1.935E+02	30	H062	1 2 2 0 0	EFG
1.771E+00	3.084E+02	50	H062	1 2 2 0 0	EFG

949. C₆H₁₄O

3-Methyl-3-pentanol

Diethylmethylcarbinol

RN: 77-74-7**MP (°C):** -24**MW:** 102.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.286E-01	4.379E+01	9.8	S307	1 1 0 2 2	
3.346E-01	3.419E+01	19.5	S307	1 1 0 2 2	
4.500E-01	4.598E+01	20	G005	1 2 1 1 2	
3.999E-01	4.086E+01	25	G005	1 2 1 1 2	
3.264E-01	3.335E+01	29.8	S307	1 1 0 2 2	
3.592E-01	3.670E+01	30	G005	1 2 1 1 2	
2.647E-01	2.705E+01	39.8	S307	1 1 0 2 2	
2.331E-01	2.382E+01	49.7	S307	1 1 0 2 2	
1.938E-01	1.980E+01	59.5	S307	1 1 0 2 2	
1.834E-01	1.874E+01	70.1	S307	1 1 0 2 2	
1.787E-01	1.826E+01	80.1	S307	1 1 0 2 2	
1.617E-01	1.652E+01	90.4	S307	1 1 0 2 2	

950. C₆H₁₄O

Dipropyl ether

Propyl ether

Dipropylaether

Dipropylether

RN: 111-43-3**MP (°C):** -123**MW:** 102.18**BP (°C):** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.644E-02	5.767E+00	0	B002	2 1 1 2 2	
3.996E-02	4.083E+00	10	B002	2 1 1 2 2	
3.705E-02	3.786E+00	15	B002	2 1 1 2 2	
2.927E-02	2.991E+00	20	B002	2 1 1 2 2	
2.936E-02	3.000E+00	20	F300	1 0 0 0 0	
6.700E-02	6.846E+00	20	S006	1 0 0 0 1	
2.441E-02	2.494E+00	25	B002	2 1 1 2 2	
1.070E-01	1.093E+01	37	E028	1 0 1 1 2	

951. C₆H₁₄O

tert-Amyl methyl ether

Methyl tert-amyl ether

RN: 994-05-8**MP (°C):****MW:** 102.18**BP (°C):** 85

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-01	1.235E+01	20	E019	1 0 1 1 2	

952. C₆H₁₄O

Propyl isopropyl ether

Propyl-isopropyl-aether

RN: 627-08-7**MP (°C):** <25**MW:** 102.18**BP (°C):** 83

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.285E-02	7.444E+00	10	B002	2 1 1 2 2	
7.242E-02	7.400E+00	10	F300	1 0 0 0 1	
5.837E-02	5.964E+00	15	B002	2 1 1 2 2	
5.872E-02	6.000E+00	15	F300	1 0 0 0 1	
4.966E-02	5.074E+00	20	B002	2 1 1 2 2	
4.578E-02	4.678E+00	25	B002	2 1 1 2 2	
4.600E-02	4.700E+00	25	F300	1 0 0 0 1	

953. C₆H₁₄O

Isohexyl alcohol

4-Methyl-1-pentanol

RN: 626-89-1 **MP (°C):** <25
MW: 102.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-01	1.042E+01	20	H330	0 0 0 0 0	

954. C₆H₁₄O

4-Methyl-2-pentanol

i-Butylmethylcarbinol

Methyl amyl alcohol

RN: 108-11-2 **MP (°C):** -90
MW: 102.18 **BP (°C):** 130

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.684E-01	2.743E+01	0	S307	1 1 0 2 2	
2.004E-01	2.047E+01	9.7	S307	1 1 0 2 2	
1.664E-01	1.701E+01	20	D052	1 1 0 0 2	
1.721E-01	1.759E+01	20	G005	1 2 1 1 2	
1.570E-01	1.604E+01	20.0	S307	1 1 0 2 2	
1.636E-01	1.672E+01	25	C093	2 1 1 1 1	
1.579E-01	1.614E+01	25	G005	1 2 1 1 2	
1.465E-01	1.497E+01	30	G005	1 2 1 1 2	
1.475E-01	1.507E+01	30.0	S307	1 1 0 2 2	
1.246E-01	1.274E+01	40.3	S307	1 1 0 2 2	
1.151E-01	1.176E+01	50.0	S307	1 1 0 2 2	
1.074E-01	1.098E+01	60.1	S307	1 1 0 2 2	
1.094E-01	1.117E+01	70.2	S307	1 1 0 2 2	
1.199E-01	1.225E+01	80.2	S307	1 1 0 2 2	
1.132E-01	1.156E+01	90.2	S307	1 1 0 2 2	

955. C₆H₁₄O

2,2-Dimethyl-3-butanol

t-Butylmethylcarbinol

RN: 464-07-3 **MP (°C):**
MW: 102.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.517E-01	2.572E+01	20	G005	1 2 1 1 2	
2.322E-01	2.372E+01	25	G005	1 2 1 1 2	
2.163E-01	2.210E+01	30	G005	1 2 1 1 2	

956. C₆H₁₄O

1-Hexanol

n-Hexanol

Amyl carbinol

Caproic alcohol

n-Hexyl alcohol**RN:** 111-27-3**MP (°C):****MW:** 102.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.173E-01	2.220E+01	0	C423	0 0 0 0 0	
7.864E-02	8.035E+00	0	E029	1 2 0 1 1	
9.344E-02	9.548E+00	0	S307	1 1 0 2 2	
1.732E-01	1.770E+01	4	C423	0 0 0 0 0	
7.706E-02	7.873E+00	5.54	H110	2 2 2 2 2	
7.487E-02	7.650E+00	6.84	H110	2 2 2 2 2	
7.213E-02	7.370E+00	8.64	H110	2 2 2 2 2	
1.223E-01	1.250E+01	10	C423	0 0 0 0 0	
6.803E-02	6.951E+00	10	E029	1 2 0 1 1	
7.372E-02	7.533E+00	10.2	S307	1 1 0 2 2	
6.906E-02	7.057E+00	11.04	H110	2 2 2 2 2	
6.671E-02	6.816E+00	12.94	H110	2 2 2 2 2	
6.506E-02	6.648E+00	14.64	H110	2 2 2 2 2	
6.287E-02	6.424E+00	17.04	H110	2 2 2 2 2	
6.861E-02	7.011E+00	20	A015	1 2 1 1 2	
6.224E-02	6.359E+00	20	E029	1 2 0 1 1	
6.070E-02	6.202E+00	20	H330	0 0 0 0 0	
4.869E-02	4.975E+00	20	L049	1 1 2 1 0	
5.150E-02	5.262E+00	20	P073	1 0 0 1 2	
6.475E-02	6.616E+00	20.0	S307	1 1 0 2 2	
5.991E-02	6.121E+00	20.74	H110	2 2 2 2 2	
5.854E-02	5.981E+00	22.94	H110	2 2 2 2 2	
6.250E-02	6.386E+00	24	H345	0 0 0 0 0	
6.069E-02	6.201E+00	25	B038	1 2 1 1 2	
5.644E-02	5.767E+00	25	B060	2 0 1 1 1	
5.837E-02	5.964E+00	25	C093	2 1 1 1 1	
7.047E-02	7.200E+00	25	C435	0 0 0 0 0	
1.000E+00	1.022E+02	25	F044	1 0 0 0 0	EFG
8.000E-02	8.174E+00	25	G075	1 0 1 0 0	
5.900E-02	6.028E+00	25	K025	2 2 1 1 2	
8.922E-02	9.116E+00	25	M323	2 2 1 1 2	
5.711E-02	5.835E+00	25.04	H110	2 2 2 2 2	
5.640E-02	5.762E+00	26.94	H110	2 2 2 2 2	
5.579E-02	5.701E+00	28.94	H110	2 2 2 2 2	
5.431E-02	5.549E+00	29.7	S307	1 1 0 2 2	
6.320E-02	6.458E+00	30	C091	1 2 1 1 1	
5.740E-02	5.865E+00	30	E029	1 2 0 1 1	
5.517E-02	5.637E+00	30.94	H110	2 2 2 2 2	
5.440E-02	5.558E+00	33.04	H110	2 2 2 2 2	
5.005E-02	5.114E+00	39.8	S307	1 1 0 2 2	
5.257E-02	5.371E+00	40	E029	1 2 0 1 1	

(continued)

956. C₆H₁₄O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.869E-02	4.975E+00	50	E029	1 2 0 1 1	
4.840E-02	4.945E+00	50.0	S307	1 1 0 2 2	
5.063E-02	5.173E+00	60	E029	1 2 0 1 1	
5.043E-02	5.153E+00	60.0	S307	1 1 0 2 2	
5.450E-02	5.569E+00	70	E029	1 2 0 1 1	
5.540E-02	5.661E+00	70	F001	1 0 1 0 2	
5.615E-02	5.737E+00	70.3	S307	1 1 0 2 2	
5.934E-02	6.063E+00	80	E029	1 2 0 1 1	
6.080E-02	6.212E+00	80	F001	1 0 1 0 2	
6.079E-02	6.211E+00	80.3	S307	1 1 0 2 2	
6.707E-02	6.853E+00	90	E029	1 2 0 1 1	
6.660E-02	6.805E+00	90	F001	1 0 1 0 2	
6.204E-02	6.340E+00	90.3	S307	1 1 0 2 2	
7.767E-02	7.937E+00	100	E029	1 2 0 1 1	
7.690E-02	7.857E+00	100	F001	1 0 1 0 2	
8.826E-02	9.018E+00	110	E029	1 2 0 1 1	
8.720E-02	8.910E+00	110	F001	1 0 1 0 2	
1.007E-01	1.029E+01	120	E029	1 2 0 1 2	
1.151E-01	1.176E+01	130	E029	1 2 0 1 2	
1.323E-01	1.351E+01	140	E029	1 2 0 1 2	
1.570E-01	1.604E+01	150	E029	1 2 0 1 2	
1.966E-01	2.009E+01	160	E029	1 2 0 1 2	
2.573E-01	2.629E+01	170	E029	1 2 0 1 2	
3.410E-01	3.484E+01	180	E029	1 2 0 1 2	
4.545E-01	4.644E+01	190	E029	1 2 0 1 2	
6.188E-01	6.323E+01	200	E029	1 2 0 1 2	
8.654E-01	8.842E+01	210	E029	1 2 0 1 2	
1.372E+00	1.402E+02	220	E029	1 2 0 1 2	
6.114E-02	6.247E+00	ns	L003	0 0 2 1 2	

957. C₆H₁₄O

2-Hexanol

n-Butylmethylcarbinol

1-Methyl pentanol

RN: 626-93-7 MP (°C): <25
 MW: 102.18 BP (°C): 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.975E-01	2.018E+01	0	S307	1 1 0 2 2	
1.617E-01	1.652E+01	10.1	S307	1 1 0 2 2	
1.246E-01	1.274E+01	19.8	S307	1 1 0 2 2	
1.456E-01	1.488E+01	20	G005	1 2 1 1 2	
1.690E-01	1.727E+01	20	H330	0 0 0 0 0	
1.323E-01	1.351E+01	25	G005	1 2 1 1 2	
1.141E-01	1.166E+01	29.9	S307	1 1 0 2 2	
1.237E-01	1.264E+01	30	G005	1 2 1 1 2	
1.055E-01	1.078E+01	40.0	S307	1 1 0 2 2	
9.306E-02	9.509E+00	50.0	S307	1 1 0 2 2	

(continued)

957. C₆H₁₄O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.826E-02	9.018E+00	60.2	S307	1 1 0 2 2	
9.498E-02	9.705E+00	70.0	S307	1 1 0 2 2	
1.094E-01	1.117E+01	80.1	S307	1 1 0 2 2	
9.114E-02	9.312E+00	90.2	S307	1 1 0 2 2	

958. C₆H₁₄O

2,2-Dimethyl-1-butanol

t-Pentylcarbinol

RN: 1185-33-7 MP (°C): -35
 MW: 102.18 BP (°C): 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.960E-02	8.133E+00	20	G005	1 2 1 1 1	
7.382E-02	7.543E+00	25	G005	1 2 1 1 1	
6.900E-02	7.050E+00	30	G005	1 2 1 1 1	

959. C₆H₁₄O

2,3-Dimethyl-1-butanol

Dimethyl-*i*-propylcarbinol

Dimethyl-isopropylcarbinol

RN: 594-60-5 MP (°C): -14
 MW: 102.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.349E-01	4.443E+01	20	G005	1 2 1 1 2	
3.927E-01	4.012E+01	25	G005	1 2 1 1 2	
3.547E-01	3.624E+01	30	G005	1 2 1 1 2	

960. C₆H₁₄O

Isopropyl ether

Diisopropyl ether

RN: 108-20-3 MP (°C): -60
 MW: 102.18 BP (°C): 68.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.351E-01	1.381E+01	24.6	H121	2 0 0 0 1	
8.730E-02	8.920E+00	25	F048	2 0 0 0 0	
7.920E-02	8.092E+00	37	E028	1 0 1 1 2	

961. C₆H₁₄O

2-Ethyl-1-butanol

2-Ethylbutanol

RN: 97-95-0

MP (°C): -15

MW: 102.18

BP (°C): 146

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.127E-02	6.261E+00	20	D052	1 1 0 0 1	
3.899E-02	3.984E+00	25	C093	2 1 1 1 0	

962. C₆H₁₄O

3-Methyl-2-pentanol

3-Methyl-2-pentyl alcohol

RN: 565-60-6 MP (°C): <25

MW: 102.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.004E-01	2.047E+01	20	G005	1 2 1 1 2	
1.863E-01	1.903E+01	25	G005	1 2 1 1 2	
1.721E-01	1.759E+01	30	G005	1 2 1 1 2	

963. C₆H₁₄O

2-Ethyl-4-butanol

3-Methylpentanol

RN: 105-30-6 MP (°C): <25

MW: 102.18 BP (°C): 148

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-01	1.284E+01	0	S307	1 1 0 2 2	
1.004E-01	1.025E+01	10.0	S307	1 1 0 2 2	
8.518E-02	8.704E+00	19.6	S307	1 1 0 2 2	
5.837E-02	5.964E+00	25	C093	2 1 1 1 1	
7.681E-02	7.848E+00	30.8	S307	1 1 0 2 2	
7.498E-02	7.661E+00	40.3	S307	1 1 0 2 2	
7.295E-02	7.454E+00	50.0	S307	1 1 0 2 2	
7.363E-02	7.523E+00	60.3	S307	1 1 0 2 2	
7.478E-02	7.641E+00	70.1	S307	1 1 0 2 2	
8.133E-02	8.310E+00	80.3	S307	1 1 0 2 2	
8.931E-02	9.126E+00	90.7	S307	1 1 0 2 2	

964. C₆H₁₄O

2-Methyl-2-pentanol

Dimethyl-*n*-propylcarbinol

1,1-Dimethyl-1-butanol

RN: 590-36-3 **MP (°C):** -107**MW:** 102.18 **BP (°C):** 122

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.428E-01	3.503E+01	20	G005	1 2 1 1 2	
3.640E-01	3.719E+01	20	H330	0 0 0 0 0	
3.071E-01	3.138E+01	25	G005	1 2 1 1 2	
2.814E-01	2.875E+01	30	G005	1 2 1 1 2	

965. C₆H₁₄O

2-Methyl-3-pentanol

i-Propylethylcarbinol**RN:** 565-67-3 **MP (°C):** <25**MW:** 102.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.144E-01	2.191E+01	20	G005	1 2 0 0 2	
1.928E-01	1.970E+01	25	G005	1 2 1 1 2	
1.749E-01	1.787E+01	30	G005	1 2 1 1 2	

966. C₆H₁₄O

3-Hexanol

n-Propylethylcarbinol*tert*-Hexyl alcohol**RN:** 623-37-0 **MP (°C):** <25**MW:** 102.18 **BP (°C):** 134.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.619E-01	2.676E+01	0	S307	1 1 0 2 2	
1.881E-01	1.922E+01	10.1	S307	1 1 0 2 2	
3.062E-01	3.129E+01	20	A015	1 2 1 1 2	
1.683E-01	1.720E+01	20	G005	1 2 1 1 2	
1.608E-01	1.643E+01	20.0	S307	1 1 0 2 2	
1.551E-01	1.584E+01	25	G005	1 2 1 1 2	
1.437E-01	1.468E+01	30	G005	1 2 1 1 2	
1.342E-01	1.371E+01	30.0	S307	1 1 0 2 2	
1.189E-01	1.215E+01	39.8	S307	1 1 0 2 2	
1.065E-01	1.088E+01	50.0	S307	1 1 0 2 2	
9.882E-02	1.010E+01	60.1	S307	1 1 0 2 2	
9.882E-02	1.010E+01	70.2	S307	1 1 0 2 2	
1.036E-01	1.059E+01	80.2	S307	1 1 0 2 2	
1.065E-01	1.088E+01	90.3	S307	1 1 0 2 2	

967. C₆H₁₄O

3-Methyl-1-pentanol

3-Methylpentanol

2-Ethyl-4-butanol

RN: 589-35-5**MP (°C):****MW:** 102.18**BP (°C):** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.190E-02	4.282E+00	25	B060	2 0 1 1 1	

968. C₆H₁₄O₂

Acetal

Acetaldehyd-diaethylacetal

Acetaldehyde diethyl acetal

RN: 105-57-7**MP (°C):****MW:** 118.18**BP (°C):** 102.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.723E-01	4.400E+01	25	F300	1 0 0 0 1	

969. C₆H₁₄O₂

Diethyl cellosolve

Ethylene glycol diethyl ether

1,2-Dieethoxyethane

3,6-Dioxaoctane

Ethyl glyme

Diethoxymethane

RN: 629-14-1**MP (°C):****MW:** 118.18**BP (°C):** 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.273E-01	2.686E+01	20	D052	1 1 0 0 2	
1.469E+00	1.736E+02	20	M062	1 0 0 0 2	

970. C₆H₁₄O₃

Carbitol

2-(2-Ethoxyethoxy)ethanol

RN: 111-90-0**MP (°C):****MW:** 134.18**BP (°C):** 196.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.610E+00	4.843E+02	4.50	C022	1 2 0 0 2	

971. C₆H₁₄O₆

D-Mannitol

1,2,3,4,5,6-Hexanehexol

Cordycepic acid

Diosmol

D-Mannite

Manna sugar

RN: 69-65-8 **MP (°C):** 167–170**MW:** 182.17 **BP (°C):** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.148E+00	2.092E+02	ns	R427	0 0 0 0 0	

972. C₆H₁₄O₆

Galactitol

Dulcit

Dulcitol

RN: 608-66-2 **MP (°C):** 189.5**MW:** 182.17 **BP (°C):** 277.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.599E-01	2.913E+01	14	D041	1 0 0 0 1	
1.702E-01	3.100E+01	15	F300	1 0 0 0 1	
2.086E+00	3.800E+02	100	F300	1 0 0 0 1	

973. C₆H₁₄O₆

Sorbitol

D-Sorbitol

RN: 50-70-4 **MP (°C):** 110**MW:** 182.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.522E+00	6.416E+02	10	M043	1 0 0 0 2	
3.785E+00	6.894E+02	20	M043	1 0 0 0 2	
4.025E+00	7.333E+02	30	M043	1 0 0 0 2	
4.283E+00	7.802E+02	40	M043	1 0 0 0 2	

974. C₆H₁₄O₆

Mannitol

D-Mannit

D-Mannitol

RN: 87-78-5 **MP (°C):** 167**MW:** 182.17 **BP (°C):** 292

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.081E-01	9.256E+01	0	C073	1 2 2 1 2	
5.171E-01	9.420E+01	0	M043	1 0 0 0 2	

(continued)

974. C₆H₁₄O₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.614E-01	1.205E+02	10	M043	1 0 0 0 2	
7.734E-01	1.409E+02	15	C073	1 2 2 1 2	
7.740E-01	1.410E+02	15	F300	1 0 0 0 2	
7.408E-01	1.349E+02	18	D041	1 0 0 0 2	
7.936E-01	1.446E+02	19	N051	1 0 2 2 2	
8.609E-01	1.568E+02	20	M043	1 0 0 0 2	
7.571E-01	1.379E+02	21.6	Y412	0 0 0 0 0	
9.762E-01	1.778E+02	25	B106	1 2 2 2 2	
9.732E-01	1.773E+02	25	B106	1 2 2 2 2	
9.739E-01	1.774E+02	25	B106	1 2 2 2 2	
9.639E-01	1.756E+02	25	C073	1 2 2 1 2	
8.255E-01	1.504E+02	25	H087	1 0 2 1 2	
8.373E-01	1.525E+02	26.8	Y412	0 0 0 0 0	
1.000E+00	1.822E+02	30	D011	1 0 1 0 1	
1.105E+00	2.013E+02	30	M043	1 0 0 0 2	
9.149E-01	1.667E+02	30.8	Y412	0 0 0 0 0	
1.254E+00	2.284E+02	35	C073	1 2 2 1 2	
9.899E-01	1.803E+02	35.6	Y412	0 0 0 0 0	
1.062E+00	1.935E+02	38.1	Y412	0 0 0 0 0	
1.411E+00	2.571E+02	40	M043	1 0 0 0 2	
1.133E+00	2.063E+02	41.8	Y412	0 0 0 0 0	
1.760E+00	3.207E+02	50	C073	1 2 2 1 2	
1.827E+00	3.329E+02	51.50	B106	1 2 2 2 2	
2.083E+00	3.794E+02	60	C073	1 2 2 1 2	
2.104E+00	3.833E+02	60	F300	1 0 0 0 2	
2.150E+00	3.917E+02	60	M043	1 0 0 0 2	
2.416E+00	4.401E+02	67.40	B106	1 2 2 2 2	
2.504E+00	4.562E+02	70.50	B106	1 2 2 2 2	
2.936E+00	5.349E+02	80	M043	1 0 0 0 2	
3.015E+00	5.493E+02	82.90	B106	1 2 2 2 2	
3.253E+00	5.927E+02	88.10	B106	1 2 2 2 2	
3.299E+00	6.010E+02	90.10	B106	1 2 2 2 2	
3.590E+00	6.540E+02	98	B106	1 2 2 2 2	
3.628E+00	6.610E+02	99.30	B106	1 2 2 2 2	
3.641E+00	6.633E+02	100	M043	1 0 0 0 2	
8.757E-01	1.595E+02	rt	D021	0 0 1 1 2	

975. C₆H₁₅N

Triethylamine

Triaethylamin

RN: 121-44-8

MP (°C): -115

MW: 101.19

BP (°C): 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.778E+00	1.799E+02	17.48	K142	1 0 0 0 2	
2.754E+00	2.787E+02	17.59	K142	1 0 0 0 2	
2.754E+00	2.787E+02	17.64	K142	1 0 0 0 2	

(continued)

975. C₆H₁₅N (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.156E+00	1.170E+02	17.82	K142	1 0 0 0 2	
1.156E+00	1.170E+02	17.85	K142	1 0 0 0 2	
2.791E+00	2.824E+02	18	C088	2 2 2 2 1	
3.434E+00	3.475E+02	18.11	K142	1 0 0 0 2	
3.434E+00	3.475E+02	18.12	K142	1 0 0 0 2	
4.014E+00	4.062E+02	19.12	K142	1 0 0 0 2	
4.014E+00	4.062E+02	19.13	K142	1 0 0 0 2	
8.951E-01	9.058E+01	19.38	K142	1 0 0 0 2	
8.951E-01	9.058E+01	19.43	K142	1 0 0 0 2	
1.403E+00	1.420E+02	20	F300	1 0 0 0 2	
6.780E-01	6.861E+01	25.04	V013	2 2 2 2 2	
1.976E-01	2.000E+01	65	F300	1 0 0 0 1	

976. C₆H₁₅N*N*-Ethyl-*sec*-butylamine*sec*-Butylethylamine2-Butanamine, *N*-ethyl-

2-(Ethylamino)butane

RN: 21035-44-9 MP (°C):

MW: 101.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.155E-01	8.253E+01	25	D332	0 0 0 0 0	
6.099E-01	6.172E+01	30	D332	0 0 0 0 0	
4.202E-01	4.252E+01	40	D332	0 0 0 0 0	

977. C₆H₁₅N*N*-Ethyl-*n*-butylamine

Ethylbutylamine

N-Ethylbutan-1-amine*N*-Ethylbutylamine

RN: 13360-63-9 MP (°C): -78

MW: 101.19 BP (°C): 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E+00	1.015E+02	10	D332	0 0 0 0 0	
5.310E-01	5.373E+01	20	D332	0 0 0 0 0	
3.793E-01	3.838E+01	30	D332	0 0 0 0 0	
2.859E-01	2.893E+01	40	D332	0 0 0 0 0	

978. C₆H₁₅N

n-Dipropylamine
Dipropylamine

RN: 142-84-7 MP (°C): -63
MW: 101.19 BP (°C): 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.470E-01	5.536E+01	12.2	H038	1 2 1 1 2	
2.794E-01	2.828E+01	36.1	H038	1 2 1 1 2	
2.335E-01	2.363E+01	44.1	H038	1 2 1 1 2	
1.900E-01	1.922E+01	52.6	H038	1 2 1 1 2	

979. C₆H₁₅O₂PS₃

Thiometon
O,O-Dimethyl S-(2-ethylmercaptoethyl) dithiophosphate

RN: 640-15-3 MP (°C):
MW: 246.35 BP (°C): 104

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.118E-04	2.000E-01	20	M061	1 0 0 0 2	
8.118E-04	2.000E-01	25	M161	1 0 0 0 2	

980. C₆H₁₅O₃PS₂

Thiolo-methylmercaptophos
Thiolo-methyl demeton

RN: MP (°C):
MW: 230.29 BP (°C): 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.433E-02	3.300E+00	20	M061	1 0 0 0 2	

981. C₆H₁₅O₃PS₂

Thiono-methylmercaptophos
Thiono-methyl demeton

RN: MP (°C):
MW: 230.29 BP (°C): 74

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.433E-03	3.300E-01	20	M061	1 0 0 0 2	

982. C₆H₁₅O₄P

Triethyl phosphate

Ethyl phosphate

Phosphoric acid, triethyl ester

TEP

RN: 78-40-0 MP (°C): -56.4

MW: 182.16 BP (°C): 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.815E+00	5.128E+02	4.50	C022	1 2 0 0 2	
2.745E+00	5.000E+02	25	F300	1 0 0 0 1	
+2.69E+00	+4.90E+02	ns	S460	0 0 0 0 0	

983. C₆H₁₆FN₂OP

Mipafox

N,N'-Diisopropylphosphorodiamidic fluoride

RN: 371-86-8 MP (°C): 65

MW: 182.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.066E-01	7.407E+01	ns	M061	0 0 0 0 0	

984. C₆H₁₆N₂

1,6-Hexanediamine

Hexamethylenediamine

RN: 124-09-4 MP (°C): 42

MW: 116.21 BP (°C): 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.123E+00	7.115E+02	4.50	C022	1 2 0 0 2	

985. C₆H₁₇N₃O₁₀S

Glycine sulfate

Triglycine sulfate

RN: 513-29-1 MP (°C):

MW: 323.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.314E-01	1.071E+02	0	M043	1 0 0 0 1	
5.155E-01	1.667E+02	10	M043	1 0 0 0 1	
6.576E-01	2.126E+02	20	M043	1 0 0 0 1	
8.188E-01	2.647E+02	30	M043	1 0 0 0 1	
9.600E-01	3.103E+02	40	M043	1 0 0 0 1	
1.326E+00	4.286E+02	60	M043	1 0 0 0 1	

986. C₆H₁₈N₄

Triethylenetetramine

N,N'-bis(2-Aminoethyl)-ethylenediamine

1,8-Diamino-3,6-diazaoctane

1,4,7,10-Tetraazadecane

3,6-Diazaoctane-1,8-diamine

Triventine

RN: 112-24-3 **MP (°C):** 12
MW: 146.24 **BP (°C):** 266

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.655E+00	8.269E+02	4.50	C022	1 2 0 0 2	

987. C₆Br₆

Hexabromobenzene

RN: 87-82-1 **MP (°C):** 327
MW: 551.52 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.558E-11	4.720E-08	10	K440	0 0 0 0 0	
1.994E-10	1.100E-07	25	K440	0 0 0 0 0	
4.207E-10	2.320E-07	35	K440	0 0 0 0 0	

988. C₆Cl₄O₂

Chloranil

Tetrachloro-*p*-benzoquinone2,3,5,6-Tetrachloro-*p*-benzoquinone

2,3,5,6-Tetrachloro-2,5-cyclohexadiene-1,4-dione

Vulklor

Coversan

RN: 118-75-2 **MP (°C):** 290
MW: 245.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.017E-03	2.500E-01	rt	M161	0 0 0 0 2	

989. C₆Cl₅NO₂

Quintozene

Pentachloronitrobenzene

Avical

Eorthcicle

Quintobenzene

RN: 82-68-8**MP (°C):** >139**MW:** 295.34**BP (°C):** 328

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-06	4.430E-04	20	E308	1 2 2 1 1	
1.862E-06	5.500E-04	22	K137	1 1 2 1 0	
1.490E-06	4.400E-04	22.5	G301	0 0 0 0 0	

990. C₆Cl₆

Hexachlorobenzene

Benzene hexachloride

HCB

Hexa-chlorobenzene

RN: 118-74-1**MP (°C):** 228**MW:** 284.78**BP (°C):** 324.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-07	3.585E-05	20	B179	0 0 0 0 0	
1.721E-08	4.900E-06	20	C113	1 0 1 1 1	
2.598E-08	7.400E-06	20	H300	1 1 2 2 1	
1.896E-08	5.400E-06	20	H300	1 1 2 2 1	
2.042E-08	5.815E-06	20	K337	1 0 0 0 2	
1.380E-08	3.931E-06	22	K305	1 0 1 1 2	
1.756E-08	5.000E-06	22.5	G301	0 0 0 0 0	
1.700E-08	4.841E-06	25	B317	0 0 0 0 0	
1.650E-08	4.699E-06	25	M342	1 0 1 1 2	
2.107E-08	6.000E-06	26.70	L095	2 2 1 1 2	
<3.51E-06	<1.00E-03	30	M311	1 1 2 2 0	
7.023E-08	2.000E-05	ns	L072	0 0 0 0 1	
2.107E-08	6.000E-06	ns	L311	0 0 0 0 1	
1.650E-07	4.699E-05	ns	M308	0 0 1 1 2	
2.458E-05	7.000E-03	rt	H053	0 2 2 2 0	γ isomer

991. C₆F₆

Hexafluorobenzene

Perfluorobenzene

RN: 392-56-3

MP (°C): 3.9 C

MW: 186.06

BP (°C): 81 C at 743 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.186E-03	7.788E-01	8.30	F418	0 0 0 0 0	
3.598E-03	6.694E-01	18.20	F418	0 0 0 0 0	
3.315E-03	6.167E-01	27.81	F418	0 0 0 0 0	
3.198E-03	5.950E-01	37.66	F418	0 0 0 0 0	
3.148E-03	5.857E-01	47.35	F418	0 0 0 0 0	
3.209E-03	5.971E-01	56.61	F418	0 0 0 0 0	
3.420E-03	6.363E-01	66.60	F418	0 0 0 0 0	

992. C₇H₃Br₂NO

Bromoxynil

3,5-Dibromo-4-hydroxybenzonitrile

4-Cyano-2,6-dibromophenol

RN: 1689-84-5 MP (°C): 190

MW: 276.93 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.694E-04	1.300E-01	25	M161	1 0 0 0 2	
4.694E-04	1.300E-01	ns	M061	0 0 0 0 2	

993. C₇H₃Br₃O₂

2,4,6-Tribromobenzoic acid

2,4,6-Tribrom-benzoesaeure

RN: 633-12-5 MP (°C):

MW: 358.83 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.754E-03	3.500E+00	15	F300	1 0 0 0 1	
1.533E-02	5.500E+00	100	F300	1 0 0 0 1	

994. C₇H₃Cl₂N

Dichlobenil

2,6-Dichlorobenzonitrile

Benzonitrile, 2,6-dichloro-

RN: 1194-65-6 **MP (°C):** 145
MW: 172.01 **BP (°C):** 270

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.046E-04	1.800E-02	20	B185	0 0 0 0 0	
1.046E-04	1.800E-02	20	B200	1 0 0 1 1	
1.046E-04	1.800E-02	20	G319	0 0 0 0 0	
1.046E-04	1.800E-02	20	M161	1 0 0 0 1	
1.163E-04	2.000E-02	25	B185	0 0 0 0 0	
5.813E-05	1.000E-02	25	M061	1 0 0 0 1	
1.046E-04	1.800E-02	ns	V303	0 0 0 0 1	

995. C₇H₃Cl₃O₂

2,3,6-Trichlorobenzoic acid

2,3,6-TBA

RN: 50-31-7 **MP (°C):** 125
MW: 225.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.726E-02	8.400E+00	20	B200	1 0 0 0 1	
3.415E-02	7.700E+00	22	M161	1 0 0 0 1	

996. C₇H₃Cl₅O

Pentachlorbenzyl alcohol

Blastin

PCBA

RN: 16022-69-8 **MP (°C):**
MW: 280.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.134E-07	2.000E-04	25	M061	0 0 0 0 0	

997. C₇H₃I₂NO

Ioxynil

4-Cyano-2,6-diiodophenol

4-Hydroxy-3,5-diiodobenzonitrile

RN: 1689-83-4 **MP (°C):** 212
MW: 370.92 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.348E-04	5.000E-02	20	F311	1 2 2 2 1	
3.505E-04	1.300E-01	25	B200	1 0 0 0 2	
1.348E-04	5.000E-02	25	M161	1 0 0 0 1	

998. C₇H₃N₃O₈

2,4,6-Trinitrobenzoic acid

2,4,6-Trinitrobenzoic acid

Acide 2,4,6-trinitrobenzoïque

RN: 129-66-8 **MP (°C):** 228.7**MW:** 257.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.817E-02	2.010E+01	23	F300	1 0 0 0 2	
7.824E-02	2.012E+01	23.5	D067	1 2 0 0 2	
1.560E-01	4.012E+01	50	D067	1 2 0 0 2	
1.560E-01	4.010E+01	50	F300	1 0 0 0 2	

999. C₇H₄BrN

4-Bromobenzonitrile

p-Bromobenzonitrile

4-Bromobenzoic acid nitrile

RN: 623-00-7 **MP (°C):** 111 C**MW:** 182.03 **BP (°C):** 236 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.635E-04	1.572E-01	22	J420	0 0 0 0 0	pH 6.5

1000. C₇H₄BrNO₄

3-Bromo-2-nitrobenzoic acid

Benzoic acid, 3-bromo-2-nitro-

RN: 116529-61-4 **MP (°C):****MW:** 246.02 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.012E-02	7.410E+00	25	H089	1 2 0 0 2	
1.341E-03	3.300E-01	25	H089	1 2 0 0 1	

1001. C₇H₄BrNS

4-Bromophenyl isothiocyanate

1-Bromo-4-isothiocyanato-benzene

RN: 1985-12-2 **MP (°C):** 60.5**MW:** 214.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-05	1.156E-02	25	D019	1 1 1 1 1	

1002. C₇H₄BrNS

3-Bromophenyl isothiocyanate

1-Bromo-3-isothiocyanato-benzene

RN: 2131-59-1 MP (°C):

MW: 214.09 BP (°C): 256.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	2.441E-02	25	D019	1 1 1 1 2	
8.200E-05	1.756E-02	25	K032	2 2 0 1 1	

1003. C₇H₄ClNO₄

3-Chloro-2-nitrobenzoic acid

2-Nitro-3-chlorobenzoic acid

RN: 4771-47-5 MP (°C):

MW: 201.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.332E-03	4.700E-01	25	H089	1 2 0 0 1	

1004. C₇H₄CINO₄

4-Chloro-3-nitrobenzoic acid

3-Nitro-4-chlorobenzoic acid

RN: 96-99-1 MP (°C): 181

MW: 201.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	3.427E-01	ns	C014	0 0 0 1 1	

1005. C₇H₄ClNO₄

5-Chloro-2-nitrobenzoic acid

2-Nitro-5-chlorobenzoic acid

RN: 2516-95-2 MP (°C):

MW: 201.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.797E-02	9.670E+00	25	H089	1 2 0 0 2	

1006. C₇H₄ClNS

3-Chlorophenyl isothiocyanate

1-Chloro-3-isothiocyanato-benzene

RN: 2392-68-9 **MP (°C):**
MW: 169.63 **BP (°C):** 249.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	3.393E-02	25	D019	1 1 1 1 0	
1.120E-04	1.900E-02	25	K032	2 2 0 1 2	

1007. C₇H₄Cl₂O₂

3,5-Dichlorobenzoic acid

Benzoic acid, 3,5-dichloro-

RN: 51-36-5 **MP (°C):** 186
MW: 191.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.700E-04	1.471E-01	ns	C014	0 0 0 1 1	

1008. C₇H₄Cl₂O₂

2,6-Dichlorobenzoic acid

2,6-Dichlor-benzoesaeure

RN: 50-30-6 **MP (°C):**
MW: 191.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-02	1.414E+01	ns	C014	0 0 0 1 1	

1009. C₇H₄Cl₂O₂

2,4-Dichlorobenzoic acid

2,4-Dichlor-benzoesaeure

RN: 50-84-0 **MP (°C):**
MW: 191.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	4.775E-01	ns	C014	0 2 0 1 1	

1010. C₇H₄Cl₂O₂

3,4-Dichlorobenzoic acid

Benzoic acid, 3,4-dichloro-

RN: 51-44-5 **MP (°C):** 208
MW: 191.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	6.112E-02	ns	C014	0 0 0 1 1	

1011. C₇H₄Cl₃NO₃

Triclopyr

Garlon

(3,5,6-Trichloro-2-pyridinyl)oxyacetic acid

Crossbow turflon

RN: 55335-06-3 MP (°C): 149

MW: 256.47 BP (°C): 290

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-03	4.300E-01	ns	K138	0 0 0 0 1	

1012. C₇H₄Cl₄O

2,4,5,6-Tetrachloro-3-methyl-phenol

m-Cresol, 2,4,5,6-tetrachloro-

Phenol, 2,3,4,6-tetrachloro-5-methyl-

RN: 10460-33-0 MP (°C):

MW: 245.92 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	6.148E-03	25	B316	0 0 0 0 0	

1013. C₇H₄Cl₄O

2,3,4,5-Tetrachloroanisole

Benzene, 1,2,3,4-tetrachloro-5-methoxy-

Anisole, 2,3,4,5-tetrachloro-

RN: 938-86-3 MP (°C): 88

MW: 245.92 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.490E-06	1.350E-03	25	L348	1 2 2 1 2	

1014. C₇H₄INS

4-Iodophenyl isothiocyanate

4-Iodophenylisothiocyanate

RN: 2059-76-9 MP (°C):

MW: 261.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	2.350E-02	25	D019	1 1 1 1 1	

1015. C₇H₄INS

3-Iodophenyl isothiocyanate

m-Iodophenyl isothiocyanate

RN: 3125-73-3 **MP (°C):**
MW: 261.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-05	5.483E-03	25	K032	2 2 0 1 0	

1016. C₇H₄I₂O₃

3,5-Diiodosalicylic acid

2-Hydroxy-3,5-diiod-benzoic acid

RN: 133-91-5 **MP (°C):** 235.5
MW: 389.92 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.274E-04	1.666E-01	10	C072	1 2 1 1 2	
1.795E-03	7.000E-01	15	F300	1 0 0 0 1	
4.931E-04	1.923E-01	25	C072	1 2 1 1 2	
3.847E-03	1.500E+00	h	F300	1 0 0 0 1	

1017. C₇H₄N₂O₂S

3-Nitrophenyl isothiocyanate

m-Nitrophenylisothiocyanate

RN: 3529-82-6 **MP (°C):**
MW: 180.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-04	5.045E-02	25	K032	2 2 0 1 2	

1018. C₇H₄N₂O₆

2,4-Dinitrobenzoic acid

2,4-Dinitrobenzoic acid

RN: 610-30-0 **MP (°C):**
MW: 212.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.580E-02	1.820E+01	25	F300	1 0 0 0 2	
4.900E-02	1.039E+01	ns	C014	0 0 0 1 1	

1019. C₇H₄N₂O₆

2,6-Dinitrobenzoic acid

2,6-Dinitrobenzoesaeure

RN: 603-12-3 **MP (°C):**
MW: 212.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-02	1.612E+01	ns	C014	0 2 0 1 1	

1020. C₇H₄N₂O₆

3,4-Dinitrobenzoic acid

3,4-Dinitrobenzoesaeure

RN: 528-45-0 **MP (°C):** 166
MW: 212.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.159E-02	6.700E+00	25	F300	1 0 0 0 1	

1021. C₇H₄N₂O₆

3,5-Dinitrobenzoic acid

3,5-Dinitrobenzoesaeure

RN: 99-34-3 **MP (°C):** 205
MW: 212.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.350E-03	1.347E+00	25	K040	1 0 2 1 2	
2.923E-03	6.200E-01	25	P037	2 0 1 1 1	

1022. C₇H₄N₄O₉

2,3,5,6-Tetranitroanisol

RN: **MP (°C):**
MW: 288.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.941E-04	2.000E-01	50	F300	1 0 0 0 0	
4.165E-03	1.200E+00	100	F300	1 0 0 0 1	

1023. C₇H₄O₆

Chelidonic acid

Chelidonsaeure

RN: 99-32-1 **MP (°C):**
MW: 184.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.767E-02	1.430E+01	25	F300	1 0 0 0 2	
2.064E-01	3.800E+01	100	F300	1 0 0 0 1	

1024. C₇H₄O₇

Meconic acid

Mekonsaeure

RN: 497-59-6

MP (°C):

MW: 200.11

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.198E-02	8.400E+00	25	F300	1 0 0 0 1	
1.034E+00	2.070E+02	100	F300	1 0 0 0 2	

1025. C₇H₅BrO₂*p*-Bromobenzoic acid

4-Bromobenzoic acid

RN: 586-76-5

MP (°C): 252.0

MW: 201.03

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-04	5.600E-02	22.5	G301	0 0 0 0 0	
2.985E-04	6.000E-02	ns	B150	0 0 2 2 1	
2.885E-04	5.800E-02	ns	B150	0 0 2 2 1	
2.800E-04	5.629E-02	ns	C014	0 0 0 1 1	

1026. C₇H₅BrO₂*m*-Bromobenzoic acid

3-Bromobenzoic acid

RN: 585-76-2

MP (°C): 155

MW: 201.03

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	4.021E-01	ns	C014	0 0 0 1 1	

1027. C₇H₅ClN₄O₂

4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-(chloroacetyl)-1,5-dihydro-

RN: 96448-62-3 MP (°C):

MW: 212.60 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.174E-04	1.100E-01	22	B428	1 2 1 2 1	

1028. C₇H₅ClO₂*meta*-Chlorobenzoic acid

3-Chlorobenzoic acid

m-Chlorobenzoic acid

3-Chlor-benzoesaeure

RN: 535-80-8 MP (°C): 154

MW: 156.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.555E-04	4.000E-02	0	F300	1 0 0 0 0	
4.080E-03	6.388E-01	24.99	B391	0 0 0 0 0	
2.555E-03	4.000E-01	25	F300	1 0 0 0 0	
2.543E-03	3.982E-01	25	T066	1 0 0 0 2	
2.555E-03	4.000E-01	37	M360	1 2 1 1 2	
2.460E-03	3.852E-01	ns	O004	0 2 1 1 2	

1029. C₇H₅ClO₂*p*-Chlorobenzoic acid

4-Chlorobenzoic acid

Chloradracylic

4-Chlor-benzoesaeure

RN: 74-11-3 MP (°C): 235

MW: 156.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.748E-04	9.000E-02	22.5	G301	0 0 0 0 0	
8.000E-04	1.253E-01	24.99	B391	0 0 0 0 0	
7.026E-04	1.100E-01	25	C410	2 0 2 2 1	
4.918E-04	7.700E-02	25	F300	1 0 0 0 1	
4.639E-04	7.263E-02	25	T066	1 0 0 0 2	
7.026E-04	1.100E-01	37	M360	1 2 1 1 2	
4.918E-04	7.700E-02	ns	B150	0 0 2 2 1	
4.350E-04	6.811E-02	ns	O004	0 2 1 1 2	

1030. C₇H₅ClO₂*o*-Chlorobenzoic acid

2-Chlor-benzoesaeure

2-Chlorobenzoic acid

RN: 118-91-2 MP (°C): 142

MW: 156.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-02	3.288E+00	24.99	B391	0 0 0 0 0	
1.916E-02	3.000E+00	25	C410	2 0 2 2 1	
1.341E-02	2.100E+00	25	F300	1 0 0 0 1	
8.686E-03	1.360E+00	25	P037	2 0 1 1 2	
1.865E-02	2.920E+00	37	M360	1 2 1 1 2	
2.574E-01	4.030E+01	100	F300	1 0 0 0 2	
1.330E-02	2.082E+00	ns	C014	0 0 0 1 2	
1.362E-02	2.132E+00	ns	O004	0 2 1 1 2	

1031. C₇H₅Cl₂NO

2,6-Dichlorobenzamide

Dichlorobenzamide

BAM

RN: 2008-58-4 MP (°C): 198

MW: 190.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.421E-02	2.700E+00	22.5	G301	0 0 0 0 0	

1032. C₇H₅Cl₂NO₂

Chloramben

3-Amino-2,5-dichlorobenzoic acid

RN: 133-90-4 MP (°C): 201

MW: 206.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.398E-03	7.000E-01	25	B200	1 0 0 0 2	
3.398E-03	7.000E-01	25	M161	1 0 0 0 2	
3.398E-03	7.000E-01	ns	B185	0 0 0 0 0	

1033. C₇H₅Cl₂NS

2,6-Dichlorothiobenzamide

Prefix

Chlorthiamid

RN: 1918-13-4 MP (°C): 151.5

MW: 206.09 BP (°C): 0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.561E-03	9.400E-01	20	M061	1 0 0 0 2	
4.610E-03	9.500E-01	21	M161	1 0 0 0 2	

1034. C₇H₅Cl₃O

2,3,4-Trichloroanisole

1,2,3-Trichloro-4-methoxy-benzene

RN: 54135-80-7 MP (°C): 70

MW: 211.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.107E-05	1.080E-02	25	L348	1 2 2 1 2	

1035. C₇H₅Cl₃O

2,4,6-Trichloro-3-methylphenol

m-Cresol, 2,4,6-trichloro-2,4,6-Trichloro-*m*-cresol

RN: 551-76-8 MP (°C):

MW: 211.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	1.121E-01	25	B316	0 0 0 0 0	

1036. C₇H₅Cl₃O

2,4,6-Trichloroanisole

1-Methoxy-2,4,6-trichlorobenzene

Methyl 2,4,6-trichlorophenyl ether

Tyrone

RN: 87-40-1 MP (°C): 61

MW: 211.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-05	1.320E-02	25	L348	1 2 2 1 2	

1037. C₇H₅FO₂*m*-Fluorobenzoic acid

3-Fluor-benzoësaeure

3-Fluorobenzoic acid

RN: 455-38-9 MP (°C): 123

MW: 140.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.071E-02	1.500E+00	25	F300	1 0 0 0 1	

1038. C₇H₅FO₂*o*-Fluorobenzoic acid

2-Fluorobenzoic acid

RN: 445-29-4 MP (°C): 123

MW: 140.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.139E-02	7.200E+00	25	F300	1 0 0 0 1	
5.129E-02	7.186E+00	ns	R427	0 0 0 0 0	

1039. C₇H₅FO₂*p*-Fluorobenzoic acid

4-Fluor-benzoësaeure

4-Fluorobenzoic acid

RN: 456-22-4 MP (°C): 182.6

MW: 140.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.564E-03	1.200E+00	25	F300	1 0 0 0 1	

1040. C₇H₅F₃N₂O₄S

3-Trifluoromethyl-4-nitrobenzenesulfonamide

4-Nitro-3-(trifluoromethyl)benzenesulfonamide

RN: 21988-05-6 MP (°C):

MW: 270.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-04	1.756E-01	15	K024	1 2 1 1 2	

1041. C₇H₅IO₂*p*-Iodobenzoic acid

4-Iodobenzoic acid

RN: 619-58-9 MP (°C):

MW: 248.02 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.120E-04	2.778E-02	15	D008	1 0 1 1 2	intrinsic

1042. C₇H₅IO₂*o*-Iodobenzoic acid

2-Iodobenzoic acid

RN: 88-67-5 MP (°C): 162

MW: 248.02 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.860E-03	4.613E-01	15	D008	1 0 1 1 2	0.002N HCl

1043. C₇H₅IO₂*m*-Iodobenzoic acid

3-Iodobenzoic acid

RN: 618-51-9 MP (°C): 187

MW: 248.02 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.380E-04	1.334E-01	15	D008	1 0 1 1 2	0.002N HCl

1044. C₇H₅I₂NO₃3,5-Diiodo-4-pyridone-*N*-acetic acid3,5-Diiodo-pyridon-(4)-*N*-essigsaeure

3,5-Diido-4-pyridone-1-acetic acid

Diodon

1,4-Dihydro-3,5-diido-4-oxopyridine-1-acetic acid

RN: 101-29-1 **MP (°C):** 244**MW:** 404.93 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.883E-03	2.787E+00	ns	H055	0 0 0 0 0	

1045. C₇H₅N

Benzonitrile

Benzonitril

Benzenenitrile

Benzoic acid nitrile

Phenyl cyanide

Cyanobenzene

RN: 100-47-0 **MP (°C):** -13**MW:** 103.12 **BP (°C):** 190.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.839E-02	1.896E+00	24.0	P321	0 0 0 0 0	
4.200E-02	4.331E+00	25	M327	1 0 0 1 2	
3.671E-02	3.786E+00	35.5	P321	0 0 0 0 0	
5.400E-02	5.569E+00	50.0	P321	0 0 0 0 0	
4.056E-02	4.182E+00	57.0	P321	0 0 0 0 0	
5.496E-02	5.668E+00	62.5	P321	0 0 0 0 0	
8.268E-02	8.527E+00	85.0	P321	0 0 0 0 0	
8.459E-02	8.723E+00	90.5	P321	0 0 0 0 0	
9.981E-02	1.029E+01	95.5	P321	0 0 0 0 0	
9.697E-02	1.000E+01	100	F300	1 0 0 0 0	
1.065E-01	1.098E+01	101.0	P321	0 0 0 0 0	
1.339E-01	1.381E+01	116.0	P321	0 0 0 0 0	
1.920E-01	1.980E+01	127.5	P321	0 0 0 0 0	
2.171E-01	2.239E+01	142.0	P321	0 0 0 0 0	
2.888E-01	2.979E+01	148.0	P321	0 0 0 0 0	
2.834E-01	2.922E+01	149.0	P321	0 0 0 0 0	
3.873E-01	3.994E+01	160.5	P321	0 0 0 0 0	
5.747E-01	5.927E+01	164.5	P321	0 0 0 0 0	
1.373E+00	1.416E+02	201.0	P321	0 0 0 0 0	
2.937E+00	3.029E+02	211.0	P321	0 0 0 0 0	
9.696E-04	9.999E-02	ns	L055	0 0 0 0 1	

1046. C₇H₅NOS

4-Hydroxyphenyl isothiocyanate

4-Hydroxyphenylisothiocyanate

RN: 2131-60-4 MP (°C):

MW: 151.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.150E-03	3.251E-01	25	D019	1 1 1 1 2	

1047. C₇H₅NOS

3-Hydroxyphenyl isothiocyanate

m-Hydroxyphenyl isothiocyanate

RN: 3125-63-1 MP (°C):

MW: 151.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.542E+00	25	K032	2 2 0 1 2	
1.023E-02	1.547E+00	ns	R427	0 0 0 0 0	

1048. C₇H₅NO₃*m*-Nitrobenzaldehyde

3-Nitrobenzaldehyde

3-Nitro-benzaldehyd

RN: 99-61-6 MP (°C): 58

MW: 151.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.617E-05	1.000E-02	25	F300	1 0 0 0 1	
3.309E+00	5.000E+02	58.0	S118	1 2 0 1 0	
6.292E-02	9.509E+00	75.1	S118	1 2 0 1 1	
3.272E+00	4.945E+02	85.2	S118	1 2 0 1 2	
1.266E-01	1.913E+01	111.9	S118	1 2 0 1 2	
1.934E-01	2.922E+01	136.4	S118	1 2 0 1 2	
3.103E-01	4.689E+01	157.3	S118	1 2 0 1 2	
6.293E-01	9.510E+01	181.0	S118	1 2 0 1 2	
8.142E-01	1.230E+02	191.4	S118	1 2 0 1 2	
1.253E+00	1.893E+02	205.4	S118	1 2 0 1 2	
1.878E+00	2.838E+02	211.8	S118	1 2 0 1 2	

1049. C₇H₅NO₃

o-Nitrobenzaldehyde
2-Nitrobenzaldehyde
2-Nitro-benzaldehyd

RN: 552-89-6 **MP (°C):** 44
MW: 151.12 **BP (°C):** 153

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-04	2.000E-02	25	F300	1 0 0 0 1	
4.600E-02	6.951E+00	66.9	S118	1 2 0 1 1	
9.972E-02	1.507E+01	103.1	S118	1 2 0 1 1	
3.001E-01	4.535E+01	166.0	S118	1 2 0 1 1	

1050. C₇H₅NO₃

p-Nitrobenzaldehyde
4-Nitrobenzaldehyde

RN: 555-16-8 **MP (°C):** 106.5
MW: 151.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.871E-01	2.828E+01	132.4	S118	1 2 0 1 2	
5.341E-01	8.071E+01	176.5	S118	1 2 0 1 2	
1.133E+00	1.713E+02	205.4	S118	1 2 0 1 2	
1.814E+00	2.742E+02	215.5	S118	1 2 0 1 2	

1051. C₇H₅NO₃S

Saccharin
1,1-Dioxide-1,2-benzisothiazol-3-(2H)-one
3-Benzisothiazolinone 1,1-dioxide
1,2-Benzisothiazol-3(2H)-one-1,1-dioxide
Kandiset
Glucid

RN: 81-07-2 **MP (°C):** 228.8
MW: 183.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-02	4.300E+00	25	F300	1 0 0 0 1	
1.880E-01	3.444E+01	30	M015	1 0 2 1 0	EFG

1052. C₇H₅NO₄

Quinolinic acid

2,3-Pyridinedicarboxylic acid

Pyridine-2,3-dicarboxylic acid

Pyridine-2,3-dicarboxylate

RN: 89-00-9 MP (°C): 190

MW: 167.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.291E-02	5.500E+00	7	F300	1 0 0 0 1	
6.600E-02	1.103E+01	25	C104	2 2 1 1 2	
6.400E-02	1.070E+01	25	C104	2 2 1 1 2	

1053. C₇H₅NO₄*p*-Nitrobenzoic acid

4-Nitrobenzoic acid

RN: 62-23-7 MP (°C): 242.4

MW: 167.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.197E-03	2.000E-01	15	F300	1 0 0 0 2	
2.525E-03	4.220E-01	24.99	B391	0 0 0 0 0	
1.660E-03	2.774E-01	25	H071	2 2 2 1 2	
3.471E-03	5.800E-01	37	B171	2 0 1 1 2	

1054. C₇H₅NO₄*o*-Nitrobenzoic acid

2-Nitrobenzoic acid

RN: 552-16-9 MP (°C): 147.5

MW: 167.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.920E-02	6.551E+00	18	D058	1 0 1 1 2	
3.340E-02	5.582E+00	24.99	B391	0 0 0 0 0	
4.325E-02	7.228E+00	25	D058	1 0 1 1 2	
4.488E-02	7.500E+00	25	F300	1 0 0 0 1	
4.350E-02	7.270E+00	25	H071	2 2 2 1 2	
4.700E-02	7.855E+00	25	K040	1 0 2 1 2	
4.360E-02	7.287E+00	25	K053	2 2 2 2 2	
4.430E-02	7.404E+00	25	L050	2 0 1 2 2	
4.415E-02	7.378E+00	25	R016	0 0 0 0 0	
4.700E-02	7.855E+00	26.4	P043	2 0 1 1 2	

1055. C₇H₅NO₄*m*-Nitrobenzoic acid

3-Nitrobenzoic acid

RN: 121-92-6 **MP (°C):** 142.0
MW: 167.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.436E-02	2.400E+00	15	F300	1 0 0 0 1	
1.530E-02	2.557E+00	24.99	B391	0 0 0 0 0	
2.121E-02	3.545E+00	25	C076	0 0 0 0 0	
2.140E-02	3.576E+00	25	K040	1 0 2 1 2	
1.227E-02	2.050E+00	25	P037	2 0 1 1 2	
6.582E-02	1.100E+01	37	B171	2 0 1 1 2	
2.334E-02	3.900E+00	ns	B361	0 0 0 0 0	

1056. C₇H₅NO₄

Isocinchomeric acid

2,5-Pyridinedicarboxylic acid

Pyridine-2,5-dicarboxylic acid

RN: 100-26-5 **MP (°C):** 254
MW: 167.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-03	1.237E+00	25	C104	2 2 1 1 2	
7.100E-03	1.187E+00	25	C104	2 2 1 1 2	

1057. C₇H₅NO₄

Cinchomeric acid

3,4-Pyridinedicarboxylic acid

RN: 490-11-9 **MP (°C):** 256
MW: 167.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-02	2.340E+00	25	C104	2 2 1 1 2	
1.380E-02	2.306E+00	25	C104	2 2 1 1 2	

1058. C₇H₅NO₄

3,5-Pyridinedicarboxylic acid

Dinicoticinic acid

RN: 499-81-0 **MP (°C):**
MW: 167.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-03	1.070E+00	25	C104	2 2 1 1 2	

1059. C₇H₅NO₄4-Formyl-2-NO₂-phenol

RN:

MP (°C):

MW: 167.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.122E-03	1.875E-01	ns	R424	0 0 0 0 0	

1060. C₇H₅NO₄

Lutidinic acid

2,4-Pyridinedicarboxylic acid

RN: 499-80-9 MP (°C): 248

MW: 167.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-02	2.490E+00	25	C104	2 2 1 1 2	
1.480E-02	2.473E+00	25	C104	2 2 1 1 2	

1061. C₇H₅NO₅

3-Nitrosalicylic acid

3-Nitro-salicylsaeure

RN: 85-38-1 MP (°C): 128

MW: 183.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.099E-03	1.300E+00	16	F300	1 0 0 0 1	

1062. C₇H₅NO₅

5-Nitrosalicylic acid

5-Nitrosalicylsaeure

RN: 96-97-9 MP (°C): 229–230

MW: 183.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.092E-02	2.000E+00	45	F300	1 0 0 0 0	

1063. C₇H₅NS

Benzothiazole

Benzthiazol

RN: 95-16-9 MP (°C): 2

MW: 135.19 BP (°C): 231

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-02	4.275E+00	ns	S460	0 0 0 0 0	

1064. C₇H₅NS

Phenyl isothiocyanate

Isothiocyanatobenzene

Phenyl mustard oil

PITC

RN: 103-72-0 MP (°C): -21.0

MW: 135.19 BP (°C): 221.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.650E-04	8.990E-02	25	D019	1 1 1 1 2	

1065. C₇H₅N₃O₆

2,4,6-Trinitrotoluene

2,4,6-Trinitrotoluol

RN: 118-96-7 MP (°C): 80.1

MW: 227.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.843E-04	1.100E-01	.3	D065	1 2 2 1 2	
4.842E-04	1.100E-01	.3	T020	1 2 2 2 2	
4.843E-04	1.100E-01	.30	F300	1 0 0 0 1	
4.975E-04	1.130E-01	5.9	D065	1 2 2 1 2	
4.974E-04	1.130E-01	5.9	T020	1 2 2 2 2	
5.283E-04	1.200E-01	20	D065	1 2 2 1 2	
5.283E-04	1.200E-01	20.0	T020	1 2 2 2 2	
8.937E-04	2.030E-01	33.1	D065	1 2 2 1 2	
8.936E-04	2.030E-01	33.1	T020	1 2 2 2 2	
1.497E-03	3.400E-01	44.2	D065	1 2 2 1 2	
1.496E-03	3.399E-01	44.2	T020	1 2 2 2 2	
1.629E-03	3.700E-01	45	D065	1 2 2 1 2	
1.628E-03	3.699E-01	45.0	T020	1 2 2 2 2	
2.351E-03	5.340E-01	53	D065	1 2 2 1 2	
2.350E-03	5.337E-01	53.0	T020	1 2 2 2 2	
2.703E-03	6.140E-01	57.1	D065	1 2 2 1 2	
2.702E-03	6.136E-01	57.1	T020	1 2 2 2 2	
4.240E-03	9.630E-01	73.2	D065	1 2 2 1 2	
4.236E-03	9.621E-01	73.2	T020	1 2 2 2 2	
6.054E-03	1.375E+00	94.4	D065	1 2 2 1 2	
6.045E-03	1.373E+00	94.4	T020	1 2 2 2 2	
6.459E-03	1.467E+00	99.5	D065	1 2 2 1 2	
6.449E-03	1.465E+00	99.5	T020	1 2 2 2 2	
6.459E-03	1.467E+00	99.50	F300	1 0 0 0 2	
6.026E-04	1.369E-01	ns	R427	0 0 0 0 0	

1066. C₇H₅N₃O₇2,4,6-Trinitro-*m*-cresol2,4,6-Trinitro-*m*-kresol

RN: 3238-38-8 MP (°C):

MW: 243.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.226E-03	2.000E+00	15	F300	1 0 0 0 0	

1067. C₇H₅N₃O₇

Methyl picric acid

2,4,6-Trinitro-3-methylphenol

3-Methyl-2,4,6-trinitrophenol

2,4,6-Trinitro-*m*-cresol

RN: 602-99-3 MP (°C):

MW: 243.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	2.431E+00	25	K053	2 2 2 2 2	

1068. C₇H₅N₃O₇

2,4,6-Trinitroanisole

2-Methoxy-1,3,5-trinitro-benzene

Methyl picrate

RN: 606-35-9 MP (°C): 69

MW: 243.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.224E-04	2.000E-01	15	D079	1 2 0 0 1	
5.627E-03	1.368E+00	50	D079	1 2 0 0 2	
1.594E-02	3.875E+00	100	D079	1 2 0 0 2	

1069. C₇H₅N₅O₈

Nitramine

Tetryl

N-Methyl-*N*,2,4,5-tetranitroaniline

RN: 479-45-8 MP (°C): 131

MW: 287.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.776E-04	5.100E-02	.5	T015	1 2 0 1 1	
1.776E-04	5.100E-02	.50	D066	1 2 2 1 2	
1.741E-04	5.000E-02	.50	F300	1 0 0 0 0	
2.403E-04	6.900E-02	9.6	D066	1 2 2 1 2	
2.403E-04	6.900E-02	9.6	T015	1 2 0 1 1	
2.473E-04	7.100E-02	14.8	D066	1 2 2 1 1	

(continued)

1069. C₇H₅N₅O₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.472E-04	7.099E-02	14.8	T015	1 2 0 1 1	
2.577E-04	7.400E-02	20.5	D066	1 2 2 1 1	
2.577E-04	7.399E-02	20.5	T015	1 2 0 1 1	
2.925E-04	8.400E-02	30	D066	1 2 2 1 1	
2.925E-04	8.399E-02	30.0	T015	1 2 0 1 1	
3.274E-04	9.400E-02	35	D066	1 2 2 1 1	
3.273E-04	9.399E-02	35.0	T015	1 2 0 1 1	
3.726E-04	1.070E-01	40	D066	1 2 2 1 2	
3.726E-04	1.070E-01	40.0	T015	1 2 0 1 2	
4.701E-04	1.350E-01	45	D066	1 2 2 1 2	
4.701E-04	1.350E-01	45.0	T015	1 2 0 1 2	
6.965E-04	2.000E-01	50	D066	1 2 2 1 2	
6.964E-04	2.000E-01	50.0	T015	1 2 0 1 2	
1.219E-03	3.500E-01	60	D066	0 0 0 0 0	
1.218E-03	3.499E-01	60.05	T015	1 2 0 1 2	
1.543E-03	4.430E-01	65	D065	1 2 2 1 2	
1.542E-03	4.428E-01	65.05	T015	1 2 0 1 2	
1.849E-03	5.310E-01	69.5	D065	1 2 2 1 2	
1.848E-03	5.307E-01	69.5	T015	1 2 0 1 2	
3.315E-03	9.520E-01	84.2	D065	1 2 2 1 2	
3.312E-03	9.511E-01	84.2	T015	1 2 0 1 2	
5.638E-03	1.619E+00	96.7	D065	1 2 2 1 2	
5.629E-03	1.616E+00	96.7	T015	1 2 0 1 2	
6.112E-03	1.755E+00	98.5	D065	1 2 2 1 2	
6.101E-03	1.752E+00	98.55	T015	1 2 0 1 2	
6.129E-03	1.760E+00	99	F300	1 0 0 0 2	

1070. C₇H₆ClF

2-Fluorobenzyl chloride

o-Fluorobenzyl chloride

RN: 345-35-7

MP (°C):

MW: 144.58

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.880E-03	4.164E-01	25	M342	1 0 1 1 2	
2.877E-03	4.160E-01	ns	S460	0 0 0 0 0	

1071. C₇H₆ClF

3-Fluorobenzyl chloride

m-Fluorobenzyl chloride

RN: 456-42-8

MP (°C):

MW: 144.58

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-03	4.135E-01	25	M342	1 0 1 1 2	
2.858E-03	4.131E-01	ns	S460	0 0 0 0 0	

1072. C₇H₆ClF

4-Fluorobenzyl chloride
 1-(Chloromethyl)-4-fluoro-benzene
 α -Chloro-*p*-fluorotoluene

RN: 352-11-4 **MP (°C):** -18
MW: 144.58 **BP (°C):** 181.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.884E-03	4.170E-01	ns	S460	0 0 0 0 0	

1073. C₇H₆ClN₃O₄S₂

Chlorothiazide

Diuresal

RN: 58-94-6 **MP (°C):** 342
MW: 295.72 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.560E-04	2.827E-01	25	A076	1 0 1 1 2	
9.000E-04	2.662E-01	30	A089	2 0 1 1 0	EFG
9.000E-04	2.662E-01	30	A093	2 0 1 1 0	EFG
6.763E-04	2.000E-01	ns	C114	0 0 0 0 0	
7.439E-04	2.200E-01	rt	A095	0 0 2 2 1	
9.806E-04	2.900E-01	rt	B181	0 0 1 1 2	

1074. C₇H₆ClN₄O₅S₂

4-Nitroso-hydrochlorothiazide

RN: **MP (°C):** 155–156
MW: 325.73 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.368E-04	2.400E-01	25	G051	1 0 1 1 0	

1075. C₇H₆Cl₂N₂O

Chlorambenamide

3,5-Dichloroanthranilamide

Benzamide, 2-amino-3,5-dichloro-

RN: 36765-01-2 **MP (°C):** 162.5
MW: 205.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.291E-03	1.700E+00	rt	M161	0 0 0 0 1	

1076. C₇H₆Cl₂O

2,6-Dichloroanisole

Benzene, 1,3-dichloro-2-methoxy-

RN: 1984-65-2 MP (°C): 31

MW: 177.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.908E-04	1.400E-01	25	L348	1 2 2 1 2	

1077. C₇H₆Cl₂O

2,3-Dichloroanisole

1,2-Dichloro-3-methoxybenzene

RN: 1984-59-4 MP (°C): 32

MW: 177.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.909E-04	8.690E-02	25	L348	1 2 2 1 2	

1078. C₇H₆Cl₂O

2,6-Dichloro-4-methyl-phenol

2,4-Dichloro-6-methyl-phenol-

RN: 2432-12-4 MP (°C):

MW: 177.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	2.833E-01	25	B316	0 0 0 0 0	
3.800E-03	6.727E-01	25	B316	0 0 0 0 0	

1079. C₇H₆N₂O₂S*p*-Cyanobenzenesulfonamide

4-Cyanobenzenesulfonamide

RN: 3119-02-6 MP (°C):

MW: 182.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-03	1.111E+00	15	K024	1 2 1 1 2	

1080. C₇H₆N₂O₄

2,4-Dinitrotoluene

2,4-Dinitro-toluol

RN: 121-14-2

MP (°C): 71

MW: 182.14

BP (°C): 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.487E-03	2.709E-01	20	T301	1 2 2 2 2	
1.482E-03	2.699E-01	22	D070	1 2 0 0 1	
1.482E-03	2.700E-01	22	F300	1 0 0 0 1	
1.482E-03	2.699E-01	22	L053	1 1 0 0 1	
2.031E-03	3.699E-01	50	D070	1 2 0 0 1	
2.031E-03	3.699E-01	50	L053	1 1 0 0 1	
1.391E-02	2.534E+00	100	D070	1 2 0 0 2	
1.449E-02	2.640E+00	100	F300	1 0 0 0 2	
1.391E-02	2.534E+00	100	L053	1 1 0 0 2	

1081. C₇H₆N₂O₅

2,4-Dinitroanisole

Dinitroanisole

Benzene, 1-methoxy-2,4-dinitro-

RN: 119-27-7

MP (°C): 88

MW: 198.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.822E-04	1.550E-01	15	D079	1 2 0 0 2	
6.863E-04	1.360E-01	50	D079	1 2 0 0 2	
2.401E-02	4.757E+00	100	D079	1 2 0 0 2	

1082. C₇H₆N₂O₅

Dinitrocresol

DNOC

2,4-Dinitro-6-methylphenol

Dinitro-*o*-cresol

RN: 534-52-1

MP (°C): 86

MW: 198.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.561E-04	1.300E-01	15	M161	1 0 0 0 2	
6.309E-04	1.250E-01	ns	B185	0 0 0 0 0	
6.459E-04	1.280E-01	ns	M061	0 0 0 0 2	
1.000E-03	1.981E-01	ns	M163	0 0 0 0 0	EFG
1.262E-03	2.500E-01	ns	N013	0 0 0 0 2	

1083. C₇H₆N₂S

4-Thiocyananiline

Rhodan

RN: 2987-46-4

MP (°C): 142

MW: 150.20

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.332E-03	2.000E-01	ns	M061	0 0 0 0 0	

1084. C₇H₆N₄

4-Methylpteridine

Pteridine, 4-methyl-

RN: 2432-21-5

MP (°C): 151

MW: 146.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.258E-01	4.762E+01	20	A083	1 2 0 0 0	

1085. C₇H₆N₄

7-Methylpteridine

Pteridine, 7-methyl-

RN: 936-40-3

MP (°C): 196.5

MW: 146.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.775E-01	1.429E+02	20	A083	1 2 0 0 0	

1086. C₇H₆N₄

2-Methylpteridine

Pteridine, 2-methyl-

RN: 2432-20-4

MP (°C): 140

MW: 146.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.842E-01	1.000E+02	20	A083	1 2 0 0 0	

1087. C₇H₆N₄O

2-Methoxypteridine

Pteridine, 2-methoxy-

RN: 102170-44-5

MP (°C): 150

MW: 162.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.614E-02	1.235E+01	20	A019	2 2 1 1 0	
1.233E+00	2.000E+02	100	A019	1 2 1 1 0	

1088. C₇H₆N₄O

4-Hydroxy-6-methylpteridine

4-Pteridinol, 6-methyl-

RN: 16041-24-0 MP (°C):

MW: 162.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.234E-02	3.623E+00	20	A019	2 2 1 1 2	
1.341E-01	2.174E+01	100	A019	1 2 1 1 1	

1089. C₇H₆N₄O

4-Hydroxy-7-methylpteridine

4-Pteridinol, 7-methyl-

RN: 34244-80-9 MP (°C):

MW: 162.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.729E-02	4.425E+00	20	A019	2 2 1 1 2	
1.713E-01	2.778E+01	100	A019	1 2 1 1 1	

1090. C₇H₆N₄O

4-Methoxypteridine

Pteridine, 4-methoxy-

RN: 30564-38-6 MP (°C): 195

MW: 162.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.614E-02	1.235E+01	20	A019	2 2 1 1 0	
6.167E-01	1.000E+02	100	A019	1 2 1 1 0	

1091. C₇H₆N₄O

7-Methoxypteridine

Pteridine, 7-methoxy-

RN: 204443-27-6 MP (°C):

MW: 162.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.209E-01	1.961E+01	20	A083	1 2 0 0 0	
1.233E+00	2.000E+02	100	A083	1 2 0 0 0	

1092. C₇H₆N₄O

3,4-Dihydro-4-keto-3-methylpteridine

3:4-Dihydro-4-keto-3-methylpteridine

RN: 24851-65-8 MP (°C): 286

MW: 162.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.686E-02	1.408E+01	20	A019	2 2 1 1 0	
6.167E-01	1.000E+02	100	A019	1 2 1 1 0	

1093. C₇H₆N₄O₂

4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-acetyl-1,5-dihydro-

RN: 96448-60-1 MP (°C):

MW: 178.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.210E-03	7.500E-01	22	B428	1 2 1 2 1	

1094. C₇H₆N₄S

7-Methylthiopteridine

Pteridine, 7-(methylthio)-

Pteridine-7-methyl-thiol

RN: 204443-30-1 MP (°C):

MW: 178.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.792E-02	4.975E+00	20	A083	1 2 0 0 0	
1.439E-01	2.564E+01	100	A083	1 2 0 0 0	

1095. C₇H₆N₄S

4-Methylthiopteridine

Pteridine, 4-(methylthio)-

Pteridine-4-methyl-thiol

RN: 6966-78-5 MP (°C): 191

MW: 178.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.313E-03	7.686E-01	20	A083	1 2 0 0 0	
3.100E-02	5.525E+00	100	A083	1 2 0 0 0	

1096. C₇H₆N₄S

4-Mercapto-7-methylpteridine

4-Pteridinethiol, 7-methyl-

RN: 98550-33-5 **MP (°C):**
MW: 178.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.738E-03	6.662E-01	100	A083	1 2 0 0 0	

1097. C₇H₆N₄S

2-Methylthiopteridine

Pteridine, 2-(methylthio)-

Pteridine-2-methyl-thiol

RN: 16878-77-6 **MP (°C):** 136
MW: 178.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.748E-02	3.115E+00	20	A083	1 2 0 0 0	
1.369E-01	2.439E+01	100	A083	1 2 0 0 0	

1098. C₇H₆O

Benzaldehyde

Benzaldehyd

RN: 100-52-7 **MP (°C):** -55
MW: 106.13 **BP (°C):** 179

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.251E-02	3.450E+00	20	C008	1 2 2 0 2	
2.827E-02	3.000E+00	20	F300	1 0 0 0 0	
3.754E-02	3.984E+00	25	B019	1 0 1 2 0	
3.754E-02	3.984E+00	25	B092	2 1 1 1 1	
6.549E-02	6.950E+00	25	C005	2 2 2 2 2	average
3.289E-02	3.490E+00	25	C008	1 2 2 0 2	
6.170E-02	6.548E+00	25	M017	1 2 0 1 2	
3.741E-02	3.970E+00	30	C008	1 2 2 0 2	
2.110E-02	2.239E+00	37	E028	1 0 1 1 2	
8.960E-02	9.509E+00	60	B092	2 0 1 1 1	

1099. C₇H₆O₂

Benzoic acid

Benzene carboxylic acid

Benzoesaeure

RN: 65-85-0**MP (°C):** 122**MW:** 122.12**BP (°C):** 249

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-02	1.697E+00	0	F302	1 0 0 0 2	
1.390E-02	1.697E+00	0	M043	1 0 0 0 1	
1.720E-02	2.100E+00	10	F300	1 0 0 0 1	
1.716E-02	2.096E+00	10	F302	1 0 0 0 2	
1.634E-02	1.996E+00	10	M043	1 0 0 0 1	
2.010E-02	2.455E+00	15	P329	0 0 0 0 0	
1.982E-02	2.421E+00	15.5	K062	2 0 1 1 2	
2.200E-02	2.687E+00	17	B109	1 0 0 0 2	unit assumed, <i>sic</i>
2.237E-02	2.732E+00	17.7	K062	2 0 1 1 2	
2.260E-02	2.760E+00	18	B109	1 0 0 0 2	unit assumed, <i>sic</i>
2.211E-02	2.700E+00	18	F071	1 1 2 1 2	
2.100E-02	2.565E+00	18	H009	2 1 2 2 0	EFG, 0.01N HCl
2.211E-02	2.700E+00	18	H080	1 0 0 0 2	
2.257E-02	2.756E+00	18	L050	2 0 1 2 2	
2.211E-02	2.700E+00	18	M344	1 0 0 0 2	
2.308E-02	2.819E+00	19.0	K062	2 0 1 1 2	average of 2
2.368E-02	2.892E+00	20	D041	1 0 0 0 1	
2.339E-02	2.857E+00	20	F069	2 2 2 2 2	
2.375E-02	2.900E+00	20	F300	1 0 0 0 1	
2.368E-02	2.892E+00	20	F302	1 0 0 0 2	
2.200E-02	2.686E+00	20	M038	2 2 1 1 2	
2.368E-02	2.892E+00	20	M043	1 0 0 0 1	
2.457E-02	3.000E+00	20	M049	1 0 0 0 1	
2.400E-02	2.931E+00	20	P329	0 0 0 0 0	
2.825E-02	3.450E+00	20	W026	1 0 1 1 1	average of 2
2.540E-02	3.102E+00	22	E045	2 0 1 1 2	
2.605E-02	3.181E+00	23	E045	2 0 1 1 2	
2.807E-02	3.428E+00	24.6	W029	1 2 1 1 2	
2.620E-02	3.200E+00	25	A412	1 0 2 2 1	int
2.449E-02	2.991E+00	25	B019	1 0 1 2 0	
2.751E-02	3.359E+00	25	B085	2 1 1 1 2	
2.683E-02	3.277E+00	25	B097	2 2 1 1 2	0.01M sodium benzoate
2.800E-02	3.420E+00	25	B128	1 0 1 1 2	
2.768E-02	3.381E+00	25	B302	1 0 0 0 0	pH 2.0
2.805E-02	3.426E+00	25	D058	1 0 1 1 2	
2.746E-02	3.354E+00	25	E045	2 0 1 1 2	
2.810E-02	3.432E+00	25	F001	1 0 1 2 2	
2.784E-02	3.400E+00	25	F300	1 0 0 0 1	
2.800E-02	3.419E+00	25	H009	2 1 2 2 0	EFG, 0.01N HCl
2.784E-02	3.400E+00	25	H015	1 0 0 0 1	
2.251E-03	2.749E-01	25	H060	2 0 2 0 2	<i>sic</i>
2.760E-02	3.371E+00	25	H071	2 2 2 1 2	
2.800E-02	3.419E+00	25	H084	1 0 0 0 1	

(continued)

1099. C₇H₆O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-02	3.371E+00	25	K005	1 0 0 1 2	
2.727E-02	3.330E+00	25	K047	1 2 1 2 2	
2.760E-02	3.371E+00	25	K057	2 2 1 1 2	
2.775E-02	3.389E+00	25	K064	2 2 2 1 2	
2.781E-02	3.396E+00	25	L048	1 2 2 1 2	
2.780E-02	3.395E+00	25	L050	2 0 1 2 2	
2.596E-02	3.170E+00	25	L338	1 0 1 1 2	
2.619E-02	3.199E+00	25	M038	2 2 1 1 2	
2.702E-02	3.300E+00	25	M049	1 0 0 0 1	
2.790E-02	3.407E+00	25	M116	2 1 1 1 2	
2.160E-02	2.638E+00	25	M149	2 0 2 2 2	intrinsic
2.900E-02	3.542E+00	25	O007	1 0 2 1 2	
2.268E-02	2.770E+00	25	P037	2 0 1 1 2	
2.807E-02	3.428E+00	25	P314	0 0 0 0 0	
8.820E+00	1.077E+03	25	P329	0 0 0 0 0	
2.793E-02	3.411E+00	25	R016	0 0 0 0 0	
2.781E-02	3.396E+00	25.0	K062	2 0 1 1 2	average of 2
2.700E-02	3.297E+00	25.00	M135	1 2 1 1 2	0.01N sodium benzoate
2.781E-02	3.396E+00	25.2	C096	1 0 0 1 2	
2.833E-02	3.460E+00	26	E045	2 0 1 1 2	
2.890E-02	3.529E+00	26.4	P043	2 0 1 1 2	
3.439E-02	4.200E+00	26.70	L095	2 2 1 1 2	
2.936E-02	3.586E+00	27	E045	2 0 1 1 2	
3.146E-02	3.842E+00	28	D050	1 2 1 2 2	
3.147E-02	3.843E+00	30	B109	1 0 0 0 2	unit assumed, <i>sic</i>
3.204E-02	3.913E+00	30	B109	1 0 0 0 2	unit assumed, <i>sic</i>
3.306E-02	4.037E+00	30	B118	1 0 0 0 2	
3.000E-02	3.664E+00	30	B142	2 0 1 1 0	EFG, 0.1N H ₂ SO ₄
3.000E-02	3.664E+00	30	C077	0 0 0 0 0	
3.319E-02	4.054E+00	30	D033	2 2 1 2 2	
3.302E-02	4.033E+00	30	D061	1 0 0 0 2	
2.915E-02	3.560E+00	30	F005	1 2 2 2 2	
3.425E-02	4.182E+00	30	F302	1 0 0 0 2	
3.110E-02	3.799E+00	30	M038	2 2 1 1 2	
3.262E-02	3.984E+00	30	M043	1 0 0 0 1	
3.302E-02	4.033E+00	30	S204	2 0 1 0 2	
3.439E-02	4.200E+00	30	W026	1 0 1 1 1	average of 2
3.216E-02	3.927E+00	30.0	K062	2 0 1 1 2	average of 2
3.400E-02	4.152E+00	31	H009	2 1 2 2 0	EFG, 0.01N HCl
3.873E-02	4.730E+00	35	G052	2 1 1 1 2	
3.711E-02	4.532E+00	35	M038	2 2 1 1 2	
4.010E-02	4.897E+00	35	O007	1 0 2 1 2	
3.772E-02	4.607E+00	35	S204	2 0 1 0 2	
3.960E-02	4.836E+00	35.0	K062	2 0 1 1 2	
3.800E-02	4.641E+00	35.00	M135	1 2 1 1 2	0.01N sodium benzoate
4.201E-02	5.131E+00	37	B171	2 0 1 1 2	
3.611E-02	4.410E+00	37	F005	1 2 2 2 2	
4.200E-02	5.129E+00	37	H009	2 1 2 2 0	EFG, 0.01N HCl
3.734E-02	4.560E+00	37	M360	1 2 1 1 2	

(continued)

1099. C₇H₆O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.528E-02	5.529E+00	40	D033	2 2 1 2 2	
4.884E-02	5.964E+00	40	F302	1 0 0 0 1	
4.376E-02	5.345E+00	40	M038	2 2 1 1 2	
4.560E-02	5.569E+00	40	M043	1 0 0 0 1	
4.424E-02	5.403E+00	40	S204	2 0 1 0 2	
5.110E-02	6.241E+00	42.4	W029	1 2 1 1 2	
4.774E-02	5.830E+00	45	F005	1 2 2 2 2	
5.000E-02	6.106E+00	45	H009	2 1 2 2 0	EFG, 0.01N HCl
5.282E-02	6.451E+00	45	M038	2 2 1 1 2	
5.254E-02	6.417E+00	45	S204	2 0 1 0 2	
5.324E-02	6.502E+00	45.0	K062	2 0 1 1 2	
5.500E-02	6.717E+00	45.00	M135	1 2 1 1 2	0.01N sodium benzoate
5.463E-02	6.672E+00	45.3	S124	1 0 0 1 1	
6.878E-02	8.400E+00	50	F300	1 0 0 0 1	
6.901E-02	8.428E+00	50	F302	1 0 0 0 2	
2.107E-02	2.573E+00	50	L006	1 0 0 0 2	
6.237E-02	7.617E+00	50	S204	2 0 1 0 2	
8.032E-02	9.809E+00	53.8	S124	1 0 0 1 2	
7.048E-02	8.607E+00	55	S204	2 0 1 0 2	
8.300E-02	1.014E+01	55.40	M135	1 2 1 1 2	0.01N sodium benzoate
8.853E-02	1.081E+01	57.8	W029	1 2 1 1 2	
9.710E-02	1.186E+01	60	F302	1 0 0 0 2	
9.550E-02	1.166E+01	60	L047	1 1 2 1 2	
9.390E-02	1.147E+01	60	M043	1 0 0 0 2	
1.000E-01	1.221E+01	60.20	M135	1 2 1 1 2	0.01N sodium benzoate
1.129E-01	1.378E+01	62.5	S124	1 0 0 1 2	
1.190E-01	1.453E+01	64.60	M135	1 2 1 1 2	0.01N sodium benzoate
1.390E-01	1.698E+01	68.50	M135	1 2 1 1 2	0.01N sodium benzoate
1.527E-01	1.864E+01	69.4	S124	1 0 0 1 2	
1.424E-01	1.739E+01	70	F302	1 0 0 0 2	
1.658E-01	2.025E+01	74.1	W029	1 2 1 1 2	
1.870E-01	2.284E+01	75.10	M135	1 2 1 1 2	0.01N sodium benzoate
2.242E-01	2.739E+01	79.0	S124	1 0 0 1 2	
2.210E-01	2.699E+01	79.30	M135	1 2 1 1 2	0.01N sodium benzoate
2.192E-01	2.676E+01	80	F302	1 0 0 0 2	
2.168E-01	2.648E+01	80	M043	1 0 0 0 2	
2.540E-01	3.102E+01	82.10	M135	1 2 1 1 2	0.01N sodium benzoate
2.567E-01	3.135E+01	82.3	S124	1 0 0 1 2	
2.485E-01	3.035E+01	83.1	W029	1 2 1 1 2	
3.124E-01	3.815E+01	88.3	W029	1 2 1 1 2	
4.211E-01	5.142E+01	88.6	S124	1 0 0 1 2	
3.550E-01	4.335E+01	88.60	M135	1 2 1 1 2	0.01N sodium benzoate
3.564E-01	4.352E+01	90	F302	1 0 0 0 2	
4.342E-01	5.302E+01	91.5	W029	1 2 1 1 2	average of 3
5.214E-01	6.367E+01	95	D041	1 0 0 0 1	
5.208E-01	6.360E+01	95	F300	1 0 0 0 2	
5.214E-01	6.367E+01	95	F302	1 0 0 0 2	
4.977E-01	6.078E+01	95.3	W029	1 2 1 1 2	
5.493E-01	6.708E+01	98.6	W029	1 2 1 1 2	

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1099. C₇H₆O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.547E-01	5.553E+01	100	M043	1 0 0 0 2	
8.241E-01	1.006E+02	109.4	W029	1 2 1 1 2	
1.399E+00	1.709E+02	116.1	W029	1 2 1 1 2	
2.594E+00	3.168E+02	116.3	W029	1 2 1 1 2	
2.001E+00	2.444E+02	117.2	W029	1 2 1 1 2	
9.000E-04	1.099E-01	ns	D037	1 1 1 1 0	pH 3.0, intrinsic

1100. C₇H₆O₂*m*-Hydroxybenzaldehyde

3-Hydroxy-benzaldehyd

RN: 100-83-4 MP (°C): 104
 MW: 122.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.252E-01	2.750E+01	43	F300	1 0 0 0 2	

1101. C₇H₆O₂*p*-Hydroxybenzaldehyde

4-Hydroxy-benzaldehyd

RN: 123-08-0 MP (°C): 213.5
 MW: 122.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.056E-01	1.290E+01	30	F300	1 0 0 0 2	

1102. C₇H₆O₂

Salicylaldehyde

Salicylaldehyd

RN: 90-02-8 MP (°C): -7
 MW: 122.12 BP (°C): 197

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.614E-04	8.077E-02	25	K129	2 1 2 2 2	
1.392E-01	1.700E+01	86	F300	1 0 0 0 1	

1103. C₇H₆O₃

Salicylic acid

2-Hydroxybenzoic acid

o-Hydroxybenzoic acid

RN: 69-72-7**MP (°C):** 158**MW:** 138.12**BP (°C):** 211

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.799E-03	9.391E-01	0	C083	1 2 1 1 2	
5.792E-03	8.000E-01	0	F300	1 0 0 0 0	
9.400E-03	1.298E+00	0	M043	1 0 0 0 0	
9.400E-03	1.298E+00	0	M043	1 0 0 0 1	
9.472E-03	1.308E+00	10	B074	1 2 1 2 2	
8.688E-03	1.200E+00	10	F300	1 0 0 0 1	
1.084E-02	1.498E+00	10	M043	1 0 0 0 0	
1.084E-02	1.498E+00	10	M043	1 0 0 0 1	
8.656E-03	1.196E+00	10	N420	0 0 0 0 0	
9.327E-03	1.288E+00	10	W044	1 0 1 0 2	
1.108E-02	1.531E+00	9.99	A341	0 0 0 0 0	
1.009E-02	1.393E+00	12.1	W044	1 0 1 0 2	
1.207E-02	1.667E+00	14.5	D061	1 0 0 0 2	
1.209E-02	1.670E+00	14.50	B118	1 0 0 0 2	unit assumed
1.028E-02	1.420E+00	15	H022	1 2 2 2 2	
1.520E-03	2.100E-01	15	M461	0 0 0 0 0	
9.875E-03	1.364E+00	15	N420	0 0 0 0 0	
1.258E-02	1.737E+00	17	K046	1 0 0 0 2	spray-dried product
1.330E-02	1.837E+00	20	B074	1 2 1 2 2	
1.303E-02	1.800E+00	20	F071	1 1 2 1 2	
1.303E-02	1.800E+00	20	F300	1 0 0 0 1	
1.303E-02	1.800E+00	20	H080	1 0 0 0 2	
1.296E-02	1.790E+00	20	K047	1 2 1 2 2	
1.445E-02	1.996E+00	20	M043	1 0 0 0 1	
1.445E-02	1.996E+00	20	M043	1 0 0 0 0	
1.445E-02	1.996E+00	20	M107	2 2 1 1 0	EFG
1.303E-02	1.800E+00	20	M344	1 0 0 0 2	
1.154E-02	1.594E+00	20	N420	0 0 0 0 0	
1.593E-02	2.200E+00	20	W026	1 0 1 1 1	average of 2
1.330E-02	1.837E+00	20	W044	1 0 1 0 2	
1.520E-02	2.100E+00	21	B331	1 2 2 1 0	pH 7.4
1.390E-02	1.920E+00	22	E045	2 0 1 1 2	
1.470E-02	2.030E+00	23	E045	2 0 1 1 2	
1.474E-02	2.036E+00	23.0	W044	1 0 1 0 2	
1.550E-02	2.141E+00	24	E045	2 0 1 1 2	
1.847E-02	2.551E+00	24.99	A341	0 0 0 0 0	
1.590E-02	2.196E+00	25	B090	1 1 1 1 2	
1.633E-02	2.255E+00	25	C083	1 2 1 1 2	
1.630E-02	2.251E+00	25	E045	2 0 1 1 2	
1.593E-02	2.200E+00	25	H007	0 0 0 0 0	
1.620E-02	2.238E+00	25	H084	1 0 0 0 2	
1.084E-02	1.498E+00	25	H129	1 0 0 1 0	

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1103. C₇H₆O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-02	2.228E+00	25	K040	1 0 2 1 2	
1.634E-02	2.257E+00	25	K053	2 2 2 2 2	
1.620E-02	2.238E+00	25	K057	2 2 1 1 2	
1.601E-02	2.211E+00	25	L050	2 0 1 2 2	
1.665E-03	2.300E-01	25	M461	0 0 0 0 0	
1.370E-02	1.892E+00	25	N420	0 0 0 0 0	
1.680E-02	2.320E+00	25	O007	1 0 2 1 2	
1.621E-02	2.239E+00	25	P314	0 0 0 0 0	
1.491E-02	2.059E+00	25.50	A012	2 2 2 2 2	
1.700E-02	2.348E+00	26	E045	2 0 1 1 2	
1.780E-02	2.459E+00	27	E045	2 0 1 1 2	
1.746E-02	2.411E+00	27	K046	1 0 0 0 2	spray-dried product
1.728E-02	2.387E+00	28	D050	1 2 1 2 2	
1.784E-02	2.464E+00	28.1	W044	1 0 1 0 2	
1.360E-02	1.878E+00	30	A065	2 0 2 2 1	
1.885E-02	2.603E+00	30	B074	1 2 1 2 2	
1.987E-02	2.745E+00	30	B118	1 0 0 0 2	unit assumed
1.750E-02	2.417E+00	30	B142	2 0 1 1 0	EFG, 0.1N H ₂ SO ₄
1.800E-02	2.486E+00	30	C077	0 0 0 0 0	
1.986E-02	2.743E+00	30	D061	1 0 0 0 2	
1.426E-02	1.970E+00	30	F005	1 2 2 2 2	
1.796E-02	2.481E+00	30	H022	1 2 2 2 2	
1.700E-02	2.348E+00	30	K020	1 0 1 1 0	EFG
1.868E-02	2.580E+00	30	K047	1 2 1 2 2	
2.022E-02	2.792E+00	30	M043	1 0 0 0 0	
2.022E-02	2.792E+00	30	M043	1 0 0 0 1	
2.165E-02	2.991E+00	30	M107	2 2 1 1 0	EFG
2.244E-03	3.100E-01	30	M461	0 0 0 0 0	
1.685E-02	2.327E+00	30	N420	0 0 0 0 0	
2.244E-02	3.100E+00	30	W026	1 0 1 1 2	average of 2
1.906E-02	2.633E+00	30	W044	1 0 1 0 2	
2.172E-02	3.000E+00	30.6	P014	2 1 2 2 0	
2.442E-02	3.373E+00	33.99	A341	0 0 0 0 0	
2.201E-02	3.041E+00	34.4	W044	1 0 1 0 2	
2.273E-02	3.140E+00	35	K047	1 2 1 2 2	
2.039E-02	2.816E+00	35	N420	0 0 0 0 0	
2.390E-02	3.301E+00	35	O007	1 0 2 1 2	
1.332E-02	1.840E+00	37	B171	2 0 1 1 2	
1.861E-02	2.570E+00	37	C079	0 0 0 0 0	
1.897E-02	2.620E+00	37	F005	1 2 2 2 2	
2.452E-02	3.386E+00	37	K046	1 0 0 0 2	spray-dried product
1.303E-02	1.800E+00	37	Y421	0 0 0 0 0	
2.590E-02	3.577E+00	38.7	W044	1 0 1 0 2	
2.848E-02	3.934E+00	40	B074	1 2 1 2 2	
2.679E-02	3.700E+00	40	F300	1 0 0 0 1	
2.672E-02	3.690E+00	40	K047	1 2 1 2 2	
3.028E-02	4.182E+00	40	M043	1 0 0 0 1	

(continued)

1103. C₇H₆O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-02	4.182E+00	40	M043	1 0 0 0 0	
2.884E-02	3.984E+00	40	M107	2 2 1 1 0	EFG
4.561E-03	6.300E-01	40	M461	0 0 0 0 0	
2.502E-02	3.456E+00	40	N420	0 0 0 0 0	
2.719E-02	3.756E+00	40	W044	1 0 1 0 2	
3.167E-02	4.374E+00	43.99	A341	0 0 0 0 0	
3.743E-02	5.170E+00	44.99	A341	0 0 0 0 0	
2.462E-02	3.400E+00	45	F005	1 2 2 2 2	
3.059E-02	4.226E+00	45	N420	0 0 0 0 0	
3.714E-02	5.130E+00	46.99	A341	0 0 0 0 0	
3.562E-02	4.921E+00	47	K046	1 0 0 0 2	spray-dried product
3.681E-02	5.084E+00	48.6	W044	1 0 1 0 2	
4.102E-02	5.665E+00	49.99	A341	0 0 0 0 0	
4.261E-02	5.885E+00	50	B074	1 2 1 2 2	
6.154E-03	8.500E-01	50	M461	0 0 0 0 0	
3.769E-02	5.206E+00	50	N420	0 0 0 0 0	
3.889E-02	5.371E+00	50	W044	1 0 1 0 2	
4.337E-02	5.991E+00	50.99	A341	0 0 0 0 0	
4.677E-02	6.461E+00	51.99	A341	0 0 0 0 0	
5.151E-02	7.115E+00	53.99	A341	0 0 0 0 0	
5.319E-02	7.347E+00	54.99	A341	0 0 0 0 0	
4.947E-02	6.833E+00	56.0	W044	1 0 1 0 2	
6.104E-02	8.431E+00	57.49	A341	0 0 0 0 0	
6.202E-02	8.566E+00	60	B074	1 2 1 2 2	
6.009E-02	8.300E+00	60	F300	1 0 0 0 1	
6.529E-02	9.018E+00	60	M043	1 0 0 0 1	
6.529E-02	9.018E+00	60	M043	1 0 0 0 0	
5.888E-02	8.133E+00	60	W044	1 0 1 0 2	
7.184E-02	9.922E+00	61.49	A341	0 0 0 0 0	
7.140E-02	9.862E+00	64.0	W044	1 0 1 0 2	
8.184E-02	1.130E+01	65.99	A341	0 0 0 0 0	
8.373E-02	1.156E+01	66.0	W044	1 0 1 0 2	
1.252E-01	1.730E+01	75.0	W044	1 0 1 0 2	
1.499E-01	2.070E+01	80	F300	1 0 0 0 2	
1.600E-01	2.210E+01	80	M043	1 0 0 0 0	
1.600E-01	2.210E+01	80	M043	1 0 0 0 2	
5.437E-01	7.510E+01	100	M043	1 0 0 0 0	
5.437E-01	7.510E+01	100	M043	1 0 0 0 2	
1.598E-02	2.207E+00	ns	O003	0 2 1 1 2	
1.514E-02	2.091E+00	ns	R427	0 0 0 0 0	
1.841E-02	2.544E+00	rt	H431	0 0 0 0 0	

1104. C₇H₆O₃

Protocatechualdehyde

3,4-Dihydroxy-benzaldehyd

RN: 139-85-5 MP (°C):

MW: 138.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.620E-01	5.000E+01	20	F300	1 0 0 0 0	
~1.88E+00	~2.60E+02	100	F300	1 0 0 0 0	

1105. C₇H₆O₃*p*-Hydroxybenzoic acid

4-Hydroxy-benzoësaeure

4-Hydroxybenzoic acid

p-Hydroxybenzoic acid

4-Hydroxybenzenecarboxylic acid

RN: 99-96-7 MP (°C): 214.5

MW: 138.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.805E-02	2.494E+00	0	M043	1 0 0 0 1	
1.590E-02	2.196E+00	4.99	A405	2 0 1 1 2	
2.525E-02	3.488E+00	10	M043	1 0 0 0 1	
2.280E-02	3.149E+00	10.99	A405	2 0 1 1 2	
2.216E-02	3.061E+00	12.7	W044	1 0 1 0 2	
5.746E-02	7.937E+00	15	D041	1 0 0 0 0	
3.186E-02	4.400E+00	15	F300	1 0 0 0 1	
2.624E-02	3.624E+00	15	H022	1 2 2 2 2	
2.990E-02	4.130E+00	15.99	A405	2 0 1 1 2	
3.740E-02	5.166E+00	19.99	A405	2 0 1 1 2	
3.470E-02	4.793E+00	20	C006	1 2 1 1 2	
3.817E-02	5.272E+00	20	M043	1 0 0 0 1	
3.602E-02	4.975E+00	20	M107	2 2 1 1 0	EFG
3.545E-02	4.896E+00	20.9	W044	1 0 1 0 2	
4.890E-02	6.754E+00	24.99	A405	2 0 1 1 2	
3.545E-02	4.896E+00	25	D081	1 1 2 1 2	
6.580E-02	9.089E+00	25	D339	0 0 0 0 0	
4.634E-02	6.400E+00	25	H007	0 0 0 0 0	
3.318E-02	4.583E+00	25	M334	1 2 1 1 2	
4.322E-02	5.970E+00	25	N023	1 2 2 1 2	hydrate
6.241E-02	8.620E+00	25	N023	1 2 2 1 2	anhydrate
3.873E-02	5.350E+00	25.50	A012	2 2 2 2 2	
6.340E-02	8.757E+00	29.99	A405	2 0 1 1 2	
5.400E-02	7.459E+00	30	A065	2 0 2 2 1	
4.800E-02	6.630E+00	30	C077	0 0 0 0 0	
5.500E-02	7.597E+00	30	H019	0 0 0 0 0	
5.421E-02	7.488E+00	30	H022	1 2 2 2 2	
5.500E-02	7.597E+00	30	K020	1 0 1 1 0	EFG (continued)

1105. C₇H₆O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.746E-02	7.937E+00	30	M043	1 0 0 0 1	
5.746E-02	7.937E+00	30	M107	2 2 1 1 0	EFG
5.538E-02	7.650E+00	30	N023	1 2 2 1 2	hydrate
7.790E-02	1.076E+01	30	N023	1 2 2 1 2	anhydride
5.496E-02	7.592E+00	30	W044	1 0 1 0 2	
8.120E-02	1.122E+01	33.99	A405	2 0 1 1 2	
7.076E-02	9.774E+00	34.4	W044	1 0 1 0 2	
7.247E-02	1.001E+01	35	N023	1 2 2 1 2	hydrate
9.781E-02	1.351E+01	35	N023	1 2 2 1 2	anhydride
1.231E-01	1.700E+01	37	B171	2 0 1 1 2	
1.027E-01	1.419E+01	38.99	A405	2 0 1 1 2	
8.663E-02	1.197E+01	39.4	W044	1 0 1 0 2	
8.938E-02	1.235E+01	40	M043	1 0 0 0 2	
9.996E-02	1.381E+01	40	M107	2 2 1 1 0	EFG
1.203E-01	1.662E+01	40	N023	1 2 2 1 2	anhydride
9.339E-02	1.290E+01	40	N023	1 2 2 1 2	hydrate
1.385E-01	1.913E+01	42.99	A405	2 0 1 1 2	
1.291E-01	1.783E+01	46.0	W044	1 0 1 0 2	
1.804E-01	2.492E+01	47.99	A405	2 0 1 1 2	
2.438E-01	3.367E+01	52.99	A405	2 0 1 1 2	
1.931E-01	2.667E+01	54.6	W044	1 0 1 0 2	
3.330E-01	4.600E+01	56.99	A405	2 0 1 1 2	
2.978E-01	4.114E+01	60	M043	1 0 0 0 2	
4.286E-01	5.920E+01	61.99	A405	2 0 1 1 2	
5.666E-01	7.826E+01	66.99	A405	2 0 1 1 2	
7.269E-01	1.004E+02	71.99	A405	2 0 1 1 2	
1.835E-01	2.534E+01	75	D041	1 0 0 0 1	
8.723E-01	1.205E+02	80	M043	1 0 0 0 2	
1.875E+00	2.590E+02	100	F300	1 0 0 0 2	
2.410E+00	3.329E+02	100	M043	1 0 0 0 2	
3.715E-02	5.132E+00	ns	R427	0 0 0 0 0	
4.854E-02	6.705E+00	rt	H431	0 0 0 0 0	

1106. C₇H₆O₃ β -2-Furyncrylic acid β -2-Furylacrylic acid β -Furyl-(2)-acrylsaeure

RN: 539-47-9

MP (°C): 143

MW: 138.12

BP (°C): 286

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.448E-02	2.000E+00	20	F300	1 0 0 0 0	

1107. C₇H₆O₃

m-Hydroxybenzoic acid
 3-Hydroxy-benzoësaeure
 3-Hydroxybenzoic acid
m-Hydroxybenzoicacid

RN: 99-06-9 **MP (°C):** 202
MW: 138.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.525E-02	3.488E+00	0	M043	1 0 0 0 1	
3.960E-02	5.470E+00	10	M043	1 0 0 0 1	
4.804E-02	6.636E+00	13.3	W044	1 0 1 0 2	
5.068E-02	7.000E+00	15	F300	1 0 0 0 1	
4.477E-02	6.184E+00	15	H022	1 2 2 2 2	
6.052E-02	8.360E+00	18.8	W044	1 0 1 0 2	
6.173E-02	8.527E+00	20	M043	1 0 0 0 1	
4.318E-02	5.964E+00	20	M107	2 2 1 1 0	EFG
7.551E-02	1.043E+01	24.3	W044	1 0 1 0 2	
5.249E-02	7.250E+00	25.50	A012	2 2 2 2 2	
7.800E-03	1.077E+00	30	A065	2 0 2 2 1	
8.600E-02	1.188E+01	30	C077	0 0 0 0 0	
8.800E-02	1.215E+01	30	H019	0 0 0 0 0	
8.300E-02	1.146E+01	30	H021	1 2 1 1 0	EFG
9.291E-02	1.283E+01	30	M043	1 0 0 0 1	
6.813E-02	9.411E+00	30	M107	2 2 1 1 0	EFG
9.552E-02	1.319E+01	30	W044	1 0 1 0 2	
9.855E-02	1.361E+01	30.9	W044	1 0 1 0 2	
1.271E-01	1.756E+01	36.2	W044	1 0 1 0 2	
1.420E-01	1.961E+01	40	M043	1 0 0 0 1	
1.105E-01	1.526E+01	40	M107	2 2 1 1 0	EFG
2.809E-01	3.880E+01	50	F300	1 0 0 0 1	
2.222E-01	3.070E+01	51.0	W044	1 0 1 0 2	
3.118E-01	4.306E+01	60	M043	1 0 0 0 1	
7.987E-01	1.103E+02	80	M043	1 0 0 0 2	
2.678E+00	3.699E+02	100	M043	1 0 0 0 2	
1.810E-02	2.500E+00	ns	B361	0 0 0 0 0	
5.012E-02	6.923E+00	ns	R427	0 0 0 0 0	

1108. C₇H₆O₄

2,6-Dihydroxybenzoic acid
 2,6-Dihydroxy-benzoësaeure
γ-Resorcylic acid

RN: 303-07-1 **MP (°C):**
MW: 154.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-02	9.556E+00	ns	C014	0 0 0 1 1	

1109. C₇H₆O₄

Protocatechuic acid

3,4-Dihydroxy-benzoesaeure

3,4-Dihydroxybenzoic acid

RN: 99-50-3 **MP (°C):****MW:** 154.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.181E-01	1.820E+01	14	F300	1 0 0 0 2	
1.440E+00	2.220E+02	80	F300	1 0 0 0 2	

1110. C₇H₆O₄

β-Resorcyclic acid

2,4-Dihydroxy-benzoesaeure

2,4-Dihydroxybenzoic acid

2,4-Dihydroxybenzoicacid

β-Resorcyclic acid

4-Hydroxysalicylic acid

RN: 89-86-1 **MP (°C):** 225**MW:** 154.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.893E-02	6.000E+00	25	H007	0 0 0 0 0	

1111. C₇H₆O₄

Gentisic acid

2,5-Dihydroxy-benzoesaeure

2,5-Dihydroxybenzoic acid

2,5-Dihydroxybenzoicacid

Hydroquinonecarboxylic acid

RN: 490-79-9 **MP (°C):** 205**MW:** 154.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.427E-01	2.200E+01	25	H007	0 0 0 0 0	

1112. C₇H₆O₅

Gallic acid

3,4,5-Trihydroxybenzoesaeure

Gallussaeure

RN: 149-91-7 **MP (°C):** 250**MW:** 170.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E+00	2.253E+02	-10.0	L430	0 0 0 0 0	
5.349E-02	9.100E+00	15	M461	0 0 0 0 0	
5.589E-02	9.509E+00	19.99	L430	0 0 0 0 0	

(continued)

1112. C₇H₆O₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.995E-02	1.190E+01	20	F300	1 0 0 0 2	
5.820E-02	9.901E+00	24.99	L430	0 0 0 0 0	
8.641E-02	1.470E+01	25	M461	0 0 0 0 0	
8.001E-02	1.361E+01	29.99	L430	0 0 0 0 0	
1.093E-01	1.860E+01	30	M461	0 0 0 0 0	
1.034E-01	1.759E+01	34.99	L430	0 0 0 0 0	
1.355E-01	2.306E+01	39.99	L430	0 0 0 0 0	
1.552E-01	2.640E+01	40	M461	0 0 0 0 0	
1.751E-01	2.979E+01	44.99	L430	0 0 0 0 0	
2.272E-01	3.865E+01	49.99	L430	0 0 0 0 0	
2.240E-01	3.810E+01	50	M461	0 0 0 0 0	
2.879E-01	4.898E+01	54.99	L430	0 0 0 0 0	
3.774E-01	6.420E+01	59.99	L430	0 0 0 0 0	
4.470E-01	7.604E+01	64.99	L430	0 0 0 0 0	
6.044E-01	1.028E+02	69.99	L430	0 0 0 0 0	
7.064E-01	1.202E+02	74.99	L430	0 0 0 0 0	
9.497E-01	1.616E+02	79.99	L430	0 0 0 0 0	
1.198E+00	2.038E+02	84.99	L430	0 0 0 0 0	
1.505E+00	2.561E+02	100	F300	1 0 0 0 2	
4.202E-02	7.149E+00	-0	L430	0 0 0 0 0	
6.918E-02	1.177E+01	ns	R427	0 0 0 0 0	

1113. C₇H₆O₅

2,3,4-Trihydroxybenzoic acid

2,3,4-Trihydroxybenzoesaeure

RN: 610-02-6 MP (°C):

MW: 170.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.878E-03	1.000E+00	12.50	F300	1 0 0 0 0	

1114. C₇H₇Br

m-Bromotoluene

3-Bromotoluene

3-Methyl-1-bromobenzene

1-Bromo-3-methylbenzene

3-Bromo-1-methylbenzene

3-Methylphenyl bromide

RN: 591-17-3 MP (°C): -39.8

MW: 171.04 BP (°C): 183.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	5.131E-02	ns	O013	0 1 0 1 0	
3.020E-04	5.165E-02	ns	S460	0 0 0 0 0	

1115. C₇H₇Cl*m*-Chlorotoluene

3-Chlorotoluene

1-Chloro-3-methylbenzene

m-Tolyl chloride

RN: 108-41-8 MP (°C): -48

MW: 126.59 BP (°C): 161.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1116. C₇H₇Cl*o*-Chlorotoluene

2-Chlorotoluene

2-Chloro-1-methylbenzene

2-Methylchlorobenzene

1-Methyl-2-chlorobenzene

OCT

RN: 95-49-8 MP (°C): -36

MW: 126.59 BP (°C): 159.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1117. C₇H₇Cl*p*-Chlorotoluene

4-Chlorotoluene

p-Tolyl chloride

4-Chloro-1-methylbenzene

PCT

1-Chloro-4-methylbenzene

RN: 106-43-4 MP (°C): 8

MW: 126.59 BP (°C): 162.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.415E-04	1.065E-01	20	H118	1 1 1 1 2	
1.084E-03	1.372E-01	20	H301	0 0 0 0 0	
3.000E-04	3.798E-02	ns	O013	0 1 0 1 0	

1118. C₇H₇ClN₂O₄S

Saluamine

2-Amino-4-chloro-5-sulfamoylbenzoic acid

4-Chloro-5-sulfamylantranilic acid

Desfurylmethylfurosemide

4-Chloro-5-sulfamylantranilic acid

-Amino-5-amino sulfonyl-4-chlorobenzoic acid

RN: 3086-91-7 **MP (°C):****MW:** 250.66 **BP (°C):** 549.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.218E-03	5.560E-01	25	B405	1 1 1 2 2	Buffer pH 2.0
3.008E-03	7.540E-01	25	B405	1 1 1 2 2	

1119. C₇H₇ClN₄O₂

8-Chlorotheophylline

8-Chloro-1,3-dimethyl-2,6(1H,3H)-purinedione

RN: 85-18-7 **MP (°C):** 290**MW:** 214.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-03	6.481E-01	ns	R427	0 0 0 0 0	

1120. C₇H₇ClO

Chlorocresol

3-Methyl-4-chlorophenol

4-Chloro-3-cresol

6-Chloro-3-hydroxytoluene

3-Methyl-4-chloro-phenol-

Phenol, 4-chloro-3-methyl-

RN: 59-50-7 **MP (°C):** 67**MW:** 142.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-02	3.992E+00	25	B316	0 0 0 0 0	
3.489E-02	4.975E+00	25	R041	0 0 0 0 0	
3.647E-02	5.200E+00	ns	G024	0 0 0 0 2	

1121. C₇H₇ClO

4-Chloroanisole

p-Chloroanisole

1-Chloro-4-methoxybenzene

RN: 623-12-1 **MP (°C):** -18**MW:** 142.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.662E-03	2.370E-01	25	L348	1 2 2 1 2	

1122. C₇H₇ClO

2-Methyl-6-chloro-phenol
 2-Chloro-6-methylphenol
 6-Chloro-*o*-cresol
 3-Chloro-2-hydroxytoluene
 6-Chloro-2-methylphenol

RN: 87-64-9 **MP (°C):**
MW: 142.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	3.565E+00	25	B316	0 0 0 0 0	

1123. C₇H₇ClO

2-Methyl-4-chloro-phenol
 4-Chloro-*o*-cresol
 4-Chloro-2-methylphenol
 5-Chloro-2-hydroxytoluene

RN: 1570-64-5 **MP (°C):** 45–48
MW: 142.59 **BP (°C):** 220–225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-02	6.844E+00	25	B316	0 0 0 0 0	

1124. C₇H₇ClO

2-Chloroanisole
o-Chloroanisole

RN: 766-51-8 **MP (°C):** –27
MW: 142.59 **BP (°C):** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.437E-03	4.900E-01	25	L348	1 2 2 1 2	
3.467E-03	4.944E-01	ns	S460	0 0 0 0 0	

1125. C₇H₇ClO

3-Chloroanisole
m-Chloroanisole
 1-Chloro-3-methoxybenzene

RN: 2845-89-8 **MP (°C):** <25
MW: 142.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.648E-03	2.350E-01	25	L348	1 2 2 1 2	
1.660E-03	2.366E-01	ns	S460	0 0 0 0 0	

1126. C₇H₇Cl₂NO

Clopidol

3,5-Dichloro-2,6-dimethyl-4-pyridinol

Coyden

Methylchloropindol

RN: 2971-90-6 MP (°C):

MW: 192.05 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.083E-04	4.000E-02	ns	K138	0 0 0 0 1	

1127. C₇H₇Cl₃NO₃PS

Chlorpyrifos-methyl

Chlorpyrifos-methy

RN: 5598-13-0 MP (°C):

MW: 322.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.581E-06	1.800E-03	10	B324	0 0 0 0 0	
5.581E-06	1.800E-03	10	B324	0 0 0 0 0	
9.922E-06	3.200E-03	20	B300	2 1 1 1 2	
9.922E-06	3.200E-03	20	B324	0 0 0 0 0	
9.921E-06	3.200E-03	20	B324	0 0 0 0 0	
1.476E-05	4.760E-03	20	C053	0 0 0 0 0	
1.240E-05	4.000E-03	24	K069	2 0 0 1 1	
1.240E-05	4.000E-03	25	M161	1 0 0 0 0	
2.139E-05	6.899E-03	30	B324	0 0 0 0 0	
2.139E-05	6.900E-03	30	B324	0 0 0 0 0	
1.476E-05	4.760E-03	ns	F071	0 1 2 1 2	
1.240E-05	4.000E-03	ns	K138	0 0 0 0 1	
1.643E-05	5.300E-03	ns	M110	0 0 0 0 0	EFG

1128. C₇H₇Cl₃NO₄P

Torelle

Dimethyl 3,5,6-trichloro-2-pyridinyl phosphate

DOWCO 217

Fospirate

Phosphoric acid, dimethyl 3,5,6-trichloro-2-pyridyl ester

RN: 5598-52-7 MP (°C):

MW: 306.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.789E-04	3.000E-01	24	K069	2 0 0 1 1	

1129. C₇H₇FN₂O₃

3-Propionyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

3-Propionyl-5-fluorouracil

RN: 75410-16-1 MP (°C): 113–114

MW: 186.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E-01	3.530E+01	22	B321	0 0 0 0 0	pH 4.0
1.896E-01	3.530E+01	22	B332	1 1 0 0 1	pH 4.0
1.980E-01	3.686E+01	22	B416	2 2 1 2 1	

1130. C₇H₇FN₂O₄

3-Acetoxyethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

3-Acetoxyethyl-5-fluorouracil

RN: 73042-04-3 MP (°C): 158–159

MW: 202.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.894E-02	2.000E+01	22	B321	0 0 0 0 0	pH 4.0

1131. C₇H₇FN₂O₄

1-Acetoxyethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

1-Acetoxyethyl-5-fluorouracil

RN: 62113-41-1 MP (°C): 122–123

MW: 202.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.132E-01	4.310E+01	22	B321	0 0 0 0 0	pH 4.0

1132. C₇H₇FN₂O₄

3-Ethyoxy carbonyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

3-Ethyoxy carbonyl-5-fluorouracil

1-Ethyoxy carbonyl-5-fluorouracil

RN: 75410-27-4 MP (°C): 126–128

MW: 202.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.562E-01	7.200E+01	22	B321	0 0 0 0 0	pH 4.0
3.413E-02	6.900E+00	22	B332	1 1 0 0 1	pH 4.0

1133. C₇H₇NO

Benzamide
Benzamid
Phenyl carboxamide
Benzoic acid amide

RN: 55-21-0 **MP (°C):** 130
MW: 121.14 **BP (°C):** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.923E-02	5.964E+00	10	M043	1 0 0 0 0	
4.750E-02	5.754E+00	12	O019	1 0 0 1 2	
1.000E-01	1.211E+01	20	B139	2 1 1 1 1	
8.173E-02	9.901E+00	20	M043	1 0 0 0 1	
1.100E-01	1.333E+01	22	J037	0 0 0 0 0	
1.106E-01	1.340E+01	25	F300	1 0 0 0 2	
1.059E-01	1.283E+01	30	M043	1 0 0 0 1	
1.300E-01	1.575E+01	40	M043	1 0 0 0 1	
1.651E-01	2.000E+01	50	P064	2 0 1 1 1	
3.931E-01	4.762E+01	60	M043	1 0 0 0 0	
6.191E-01	7.500E+01	70	P064	2 0 1 1 1	
5.503E+00	6.667E+02	80	M043	1 0 0 0 2	
6.686E+00	8.100E+02	90	P064	2 0 1 1 2	
7.338E+00	8.889E+02	100	M043	1 0 0 0 2	
7.842E+00	9.500E+02	110	P064	2 0 1 1 2	
1.100E-01	1.332E+01	rt	D021	0 0 1 1 2	

1134. C₇H₇NO₂

Salicylamide
2-Hydroxybenzoicacidamide
Algamon
Amid-sal
Amidosal
Algiamida

RN: 65-45-2 **MP (°C):** 140
MW: 137.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.878E-03	1.218E+00	10	N419	0 0 0 0 0	
1.060E-02	1.454E+00	15	D012	1 1 0 1 2	
1.137E-02	1.559E+00	15	N419	0 0 0 0 0	
1.100E-02	1.509E+00	16	D012	1 1 0 1 2	
1.531E-02	2.100E+00	20	E046	1 0 0 0 0	EFG
1.447E-02	1.985E+00	20	N419	0 0 0 0 0	
1.900E-02	2.606E+00	22	J031	0 0 0 0 0	
1.604E-02	2.200E+00	23	B328	1 2 2 1 1	pH 4.0
1.500E-02	2.057E+00	25	D012	1 1 0 1 2	
1.750E-02	2.400E+00	25	E046	1 0 0 0 0	EFG
1.757E-02	2.409E+00	25	N419	0 0 0 0 0	
1.831E-02	2.511E+00	25	P314	0 0 0 0 0	

(continued)

1134. C₇H₇NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.115E-02	2.900E+00	30	E046	1 0 0 0 0	EFG
2.166E-02	2.970E+00	30	N419	0 0 0 0 0	
2.771E-02	3.800E+00	35	E046	1 0 0 0 0	EFG
2.685E-02	3.682E+00	35	N419	0 0 0 0 0	
2.900E-02	3.977E+00	37	D012	1 1 0 1 2	
3.427E-02	4.700E+00	40	E046	1 0 0 0 0	EFG
3.285E-02	4.505E+00	40	N419	0 0 0 0 0	
4.280E-02	5.870E+00	45	D012	1 1 0 1 2	
4.181E-02	5.734E+00	45	N419	0 0 0 0 0	
5.323E-02	7.300E+00	50	E046	1 0 0 0 0	EFG
5.371E-02	7.366E+00	50	N419	0 0 0 0 0	
1.677E-03	2.300E-01	ns	B361	0 0 0 0 0	

1135. C₇H₇NO₂*p*-Aminobenzoic acid

4-Amino-benzoesaeure

4-Aminobenzoic acid

p-Aminobenzoicacid

1-Amino-4-carboxybenzene

RN: 150-13-0 **MP (°C):** 187.0**MW:** 137.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.479E-02	3.400E+00	12.80	F300	1 0 0 0 1	
3.609E-02	4.950E+00	18	C033	1 0 2 1 2	
3.628E-02	4.975E+00	25	D041	1 0 0 0 0	
3.930E-02	5.390E+00	25	L338	1 0 1 1 2	
3.646E-02	5.000E+00	25	M054	1 0 0 0 0	
3.500E-02	4.800E+00	25	P015	0 0 0 0 0	
4.455E-02	6.110E+00	30	C033	1 0 2 1 2	
4.579E-02	6.280E+00	30	H018	0 0 0 0 0	
4.500E-02	6.171E+00	30	L069	1 0 1 1 0	EFG
6.125E-02	8.400E+00	37	B171	2 0 1 1 2	
6.040E-02	8.283E+00	37	F006	1 1 2 2 2	

1136. C₇H₇NO₂*o*-Nitrotoluene

2-Nitro-toluol

2-Nitrotoluene

RN: 88-72-2 **MP (°C):** -9.5**MW:** 137.14 **BP (°C):** 221.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.872E-03	5.310E-01	9.99	B403	1 2 2 2 2	
4.441E-03	6.090E-01	19.99	B403	1 2 2 2 2	

(continued)

1136. C₇H₇NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.017E-03	6.880E-01	29.99	B403	1 2 2 2 2	
4.740E-03	6.500E-01	30	F300	1 0 0 0 2	
5.637E-03	7.730E-01	39.99	B403	1 2 2 2 2	

1137. C₇H₇NO₂*o*-Aminobenzoic acid

2-Aminobenzoic acid

Anthranilsaeure

RN: 118-92-3 MP (°C): 145

MW: 137.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.181E-02	2.991E+00	10	M043	1 0 0 0 0	
2.543E-02	3.488E+00	14	D041	1 0 0 0 1	
2.552E-02	3.500E+00	14	F300	1 0 0 0 1	
2.543E-02	3.488E+00	20	M043	1 0 0 0 1	
4.349E-02	5.964E+00	30	M043	1 0 0 0 0	
6.504E-02	8.920E+00	40	M043	1 0 0 0 0	
3.552E+00	4.872E+02	100	M043	1 0 0 0 1	

1138. C₇H₇NO₂*m*-Nitrotoluene

3-Nitro-toluol

3-Nitrotoluene

RN: 99-08-1 MP (°C): 16

MW: 137.14 BP (°C): 232.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.281E-03	4.500E-01	9.99	B403	1 2 2 2 2	
3.580E-03	4.910E-01	19.99	B403	1 2 2 2 2	
3.894E-03	5.340E-01	29.99	B403	1 2 2 2 2	
3.646E-03	5.000E-01	30	F300	1 0 0 0 2	
4.120E-03	5.650E-01	39.99	B403	1 2 2 2 2	

1139. C₇H₇NO₂*m*-Aminobenzoic acid

3-Amino-benzoesaeure

3-Aminobenzoic acid

RN: 99-05-8 MP (°C): 174

MW: 137.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.302E-02	5.900E+00	14.90	F300	1 0 0 0 1	
5.830E-02	7.995E+00	30	W007	2 0 2 2 2	

1140. C₇H₇NO₂

Methyl nicotinate

Nicotinsaeure-methyl ester

RN: 93-60-7

MP (°C): 39

MW: 137.14

BP (°C): 209

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.471E-01	4.760E+01	20	F300	1 0 0 0 2	<i>sic</i>
8.065E+00	1.106E+03	32	L346	1 0 0 1 0	
3.467E-01	4.755E+01	ns	R424	0 0 0 0 0	

1141. C₇H₇NO₂*p*-Nitrotoluene

4-Nitrotoluene

RN: 99-99-0

MP (°C): 55

MW: 137.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.305E-03	1.790E-01	9.99	B403	1 2 2 2 2	
2.917E-04	4.000E-02	14.5	D070	1 2 0 0 1	
2.917E-04	4.000E-02	14.50	F300	1 0 0 0 1	
1.765E-03	2.420E-01	19.99	B403	1 2 2 2 2	
2.100E-03	2.880E-01	20	H306	1 0 1 2 1	
2.150E-03	2.949E-01	20	T301	1 2 2 2 2	
2.348E-03	3.220E-01	29.99	B403	1 2 2 2 2	
3.048E-03	4.180E-01	39.99	B403	1 2 2 2 2	
5.687E-04	7.799E-02	50	D070	1 2 0 0 1	
8.458E-04	1.160E-01	100	D070	1 2 0 0 2	

1142. C₇H₇NO₃

3-Methyl-4-nitrophenol

3-Nitro-*p*-cresol3-Nitro-*p*-kresol

4-Nitro-5-methylphenol

RN: 2581-34-2

MP (°C): 128

MW: 153.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.769E-03	1.190E+00	25	B104	1 2 1 1 1	
7.762E-03	1.189E+00	ns	R427	0 0 0 0 0	

1143. C₇H₇NO₃*p*-Aminosalicylic acid

4-Amino-salicylsaeure

4-Aminosalicylic acid

RN: 65-49-6**MP (°C):** 150**MW:** 153.14**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	1.996E+00	20	D041	1 0 0 0 0	
1.100E-02	1.685E+00	23	M072	1 2 1 1 0	EFG
2.100E-02	3.216E+00	30	L069	1 0 1 1 0	EFG
1.087E-02	1.664E+00	ns	H125	0 0 0 0 0	

1144. C₇H₇NO₃*p*-Nitroanisol

4-Nitro-anisol

4-Nitroanisol

RN: 100-17-4**MP (°C):** 54**MW:** 153.14**BP (°C):** 260

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	7.000E-02	15	F300	1 0 0 0 1	
3.853E-03	5.900E-01	30	F300	1 0 0 0 2	

1145. C₇H₇N₂OS

Ethyl acetylthiodiazole

Ethyle acetyle thioldiazolique

RN: MP (°C):**MW:** 167.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.196E-03	2.000E-01	37	D084	1 0 1 0 1	

1146. C₇H₇N₅

2-Methylaminopteridine

Pteridine, 2-(methylamino)-

RN: 19167-57-8 **MP (°C):** 219**MW:** 161.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-02	3.115E+00	20	A019	2 2 1 1 1	
1.724E-01	2.778E+01	100	A019	1 2 1 1 1	

1147. C₇H₈

Toluene

Methylbenzene

RN: 108-88-3

MP (°C): -94

MW: 92.14

BP (°C): 110.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.819E-03	5.362E-01	.06	U010	1 0 0 1 1	
7.857E-03	7.240E-01	0	P003	2 2 2 2 2	
6.638E-03	6.116E-01	4.50	B086	2 1 2 2 2	
5.557E-03	5.120E-01	4.62	U010	1 0 0 1 1	EFG
5.557E-03	5.120E-01	4.62	U013	1 0 0 0 0	EFG
6.519E-03	6.006E-01	6.30	B086	2 1 2 2 2	
6.356E-03	5.857E-01	7.10	B086	2 1 2 2 2	
6.367E-03	5.867E-01	9	B086	2 1 2 2 2	
6.210E-03	5.722E-01	10	B149	2 1 1 2 2	
6.215E-03	5.727E-01	11.80	B086	2 1 2 2 2	
6.237E-03	5.747E-01	12.10	B086	2 1 2 2 2	
5.307E-03	4.890E-01	14.20	U013	1 0 0 0 0	EFG
5.785E-03	5.330E-01	15	S203	1 1 2 1 2	
6.172E-03	5.687E-01	15.10	B086	2 1 2 2 2	
5.424E-03	4.998E-01	16	D052	1 1 0 0 0	
5.100E-03	4.699E-01	16	F001	1 0 1 2 1	
5.101E-03	4.700E-01	16	F071	1 1 2 1 2	
5.101E-03	4.700E-01	16	F300	1 0 0 0 2	
5.101E-03	4.700E-01	16	H080	1 0 0 0 2	
5.100E-03	4.699E-01	16	S006	1 0 0 0 1	
6.370E-03	5.869E-01	20	B149	2 1 1 2 2	
6.154E-03	5.670E-01	20	B356	0 0 0 0 0	
5.424E-03	4.998E-01	20	C121	1 0 0 0 0	unit assumed, <i>sic</i>
5.590E-03	5.151E-01	20	M312	1 0 0 0 2	
4.982E-03	4.591E-01	20	M337	2 1 2 2 2	
6.139E-03	5.657E-01	20.10	B086	2 1 2 2 2	
5.196E-03	4.788E-01	21	C024	2 1 1 2 2	
5.752E-03	5.300E-01	25	A001	1 2 2 2 1	
5.098E-03	4.698E-01	25	A094	1 0 0 0 1	
6.805E-03	6.270E-01	25	B003	2 1 2 2 2	
5.589E-03	5.150E-01	25	B060	2 0 1 1 1	
6.690E-03	6.164E-01	25	B153	2 1 1 1 2	
1.680E-02	1.548E+00	25	B173	2 0 2 2 2	<i>sic</i>
5.687E-03	5.240E-01	25	B304	2 0 2 2 2	
8.000E-03	7.371E-01	25	H092	1 1 1 1 0	
6.500E-03	5.989E-01	25	H313	2 1 2 2 1	
6.000E-03	5.529E-01	25	H332	2 2 2 2 0	
6.370E-02	5.869E+00	25	I334	2 2 2 1 2	<i>sic</i>
6.370E-03	5.869E-01	25	I335	2 2 2 2 2	
5.430E-03	5.003E-01	25	K001	1 0 2 1 2	
5.318E-03	4.900E-01	25	K072	1 0 1 1 1	
6.290E-03	5.796E-01	25	K316	2 2 2 2 2	
5.641E-03	5.197E-01	25	L319	1 0 2 1 2	

(continued)

1147. C₇H₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.589E-03	5.150E-01	25	M130	1 0 0 0 2	
5.638E-03	5.195E-01	25	M132	2 2 2 1 2	
6.280E-03	5.787E-01	25	M342	1 0 1 1 2	
6.219E-03	5.730E-01	25	P003	2 2 2 2 2	
6.012E-03	5.540E-01	25	P051	2 1 1 2 2	
6.045E-03	5.570E-01	25	S203	1 1 2 1 2	
5.804E-03	5.348E-01	25	S358	2 1 2 2 2	
5.650E-03	5.206E-01	25	S359	2 1 2 2 2	
6.280E-03	5.787E-01	25	W300	2 2 2 2 2	
5.307E-03	4.890E-01	25.35	U010	1 0 0 1 1	EFG
5.307E-03	4.890E-01	25.35	U013	1 0 0 0 0	EFG
3.255E-03	2.999E-01	30	F053	1 0 2 0 2	
6.183E-03	5.697E-01	30	G029	1 0 2 2 1	
5.067E-03	4.669E-01	30	M311	1 1 2 2 2	
1.409E-02	1.298E+00	30	S207	1 0 0 1 1	<i>sic</i>
5.557E-03	5.120E-01	34.53	U010	1 0 0 1 1	EFG
5.557E-03	5.120E-01	34.53	U013	1 0 0 0 0	EFG
6.371E-03	5.870E-01	35	S203	1 1 2 1 2	
5.954E-03	5.486E-01	44.30	U010	1 0 0 1 1	EFG
5.819E-03	5.362E-01	44.30	U013	1 0 0 0 0	EFG
6.892E-03	6.350E-01	45	S203	1 1 2 1 2	
1.517E-02	1.398E+00	45	S207	1 0 0 1 1	<i>sic</i>
6.529E-03	6.015E-01	54.71	U013	1 0 0 0 0	EFG
1.500E-02	1.382E+00	55	H092	1 1 1 1 1	
6.380E-03	5.879E-01	55.79	U010	1 0 0 1 1	EFG
1.734E-02	1.597E+00	60	S207	1 0 0 1 1	<i>sic</i>
7.325E-03	6.749E-01	65.82	U013	1 0 0 0 0	EFG
2.171E-02	2.000E+00	150	J023	1 1 2 2 0	
7.597E-02	7.000E+00	200	J023	1 1 2 2 0	
3.039E-01	2.800E+01	250	J023	1 1 2 2 1	
1.411E+00	1.300E+02	300	J023	1 1 2 2 2	
5.589E-03	5.150E-01	ns	H123	0 0 0 0 0	
1.380E-01	1.272E+01	ns	H307	0 0 0 0 0	<i>sic</i>
5.611E-03	5.170E-01	ns	M175	0 0 2 1 2	
5.589E-03	5.150E-01	ns	M344	0 0 0 0 2	

1148. C₇H₈

1,6-Heptadiyne

RN: 2396-63-6 **MP (°C):** -85
MW: 92.14 **BP (°C):** 112

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.791E-02	1.650E+00	25	M001	2 1 2 2 2	

1149. C₇H₈

Cycloheptatriene

1,3,5-Cycloheptatriene

Tropilidene

CHT

RN: 544-25-2**MP (°C):** -80**MW:** 92.14**BP (°C):** 116.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.301E-03	5.806E-01	4.8	L007	2 2 1 2 2	
6.301E-03	5.806E-01	5.1	L007	2 1 1 1 2	
7.207E-03	6.641E-01	14.8	L007	2 2 1 2 2	
7.207E-03	6.641E-01	15.2	L007	2 1 1 1 2	
7.260E-03	6.690E-01	24.8	L007	2 2 1 2 2	
6.729E-03	6.200E-01	25	M001	2 1 2 2 2	
7.260E-03	6.690E-01	25.1	L007	2 1 1 1 2	
8.045E-03	7.413E-01	34.8	L007	2 2 1 2 2	
8.045E-03	7.413E-01	35.2	L007	2 1 1 1 2	
8.294E-03	7.642E-01	44.8	L007	2 2 1 2 2	
8.294E-03	7.642E-01	45.2	L007	2 1 1 1 2	

1150. C₇H₈ClN₃O₄S₂

Hydrochlorothiazide

Chlorozide

RN: 58-93-5**MP (°C):** 274**MW:** 297.74**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.425E-03	7.220E-01	25	A076	1 0 1 1 2	
2.032E-03	6.050E-01	25	C437	0 0 0 0 0	Average
2.045E-03	6.090E-01	25	D091	1 0 0 0 2	pH 6.2
2.687E-03	8.000E-01	25	G051	1 0 1 1 0	
2.800E-03	8.337E-01	30	A089	2 0 1 1 0	EFG
2.800E-03	8.337E-01	30	A093	2 0 1 1 0	EFG
2.520E-03	7.503E-01	30	E049	2 0 2 2 2	
3.627E-03	1.080E+00	37	D091	1 0 0 0 2	pH 7.2
7.650E-03	2.278E+00	50	M335	1 0 2 1 2	pH 5
3.359E-03	1.000E+00	ns	K444	0 0 0 0 0	
1.982E-03	5.900E-01	rt	A095	0 0 0 0 0	

1151. C₇H₈ClN₃O₄S₂

Hydrochlorothiazide

3,4-Dihydro-6-chloro-7-sulfamoyl-1,2,4-benzothiadiazine-1,1-dioxide

3,4-Dihydrochlorothiazide

6-Chloro-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulfonamide-1,1-dioxide

6-Chloro-3,4-dihydro-7-sulfamoyl-2H-1,2,4-benzothiadiazine-1,1-dioxide

Aldactazide

RN: 58-93-5 MP (°C): 274

MW: 297.74 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.997E-03	5.946E-01	22.5	B422	2 0 2 2 2	
2.351E-06	7.000E-04	25	A408	2 0 1 2 0	
2.115E-03	6.296E-01	25	S450	0 0 0 0 0	

1152. C₇H₈FN₃O₃

1-Ethylcarbamoyl-5-fluorouracil

1-Ethylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

N-Ethyl-5-fluoro-3,4-dihydro-2,4-dioxo-1-pyrimidinecarboxamide

RN: 58471-47-9 MP (°C): 190–196

MW: 201.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.457E-03	1.500E+00	22	B321	0 0 0 0 0	pH 4.0
7.457E-03	1.500E+00	22	B388	0 0 0 0 0	

1153. C₇H₈FN₃O₃1-(*N,N*-Dimethylcarbamoyl)-5-fluorouracil

1-Dimethylcarbamoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

RN: 60908-29-4 MP (°C): 226–227

MW: 201.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.983E-02	6.000E+00	22	B321	0 0 0 0 0	pH 4.0
2.983E-02	6.000E+00	22	B388	0 0 0 0 0	

1154. C₇H₈N₂O₂3-Nitro-*o*-toluidine3-Nitro-*o*-toluidin

RN: 603-83-8 MP (°C): 92

MW: 152.15 BP (°C): 305

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.807E-02	1.340E+01	100	F300	1 0 0 0 2	

1155. C₇H₈N₂O₃

5,5-Trimethylenebarbituric acid

6,8-Diazaspiro[3.5]nonane-5,7,9-trione

Cyclobutane-spirobarbiturate

RN: 6128-03-6 MP (°C):

MW: 168.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.213E-02	3.721E+00	25	P350	0 0 0 0 0	intrinsic

1156. C₇H₈N₂O₃

1-Methoxy-2-amino-4-nitrobenzene

RN: 99-59-2 MP (°C): 118

MW: 168.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-03	5.697E-01	rt	N015	0 0 2 2 2	

1157. C₇H₈N₂O₃S

5-Carboethoxy-2-thiouracil

Ethyl 2-thiouracil-5-carboxylate

RN: 38026-46-9 MP (°C): 252

MW: 200.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.970E-03	1.596E+00	25	G016	1 2 1 2 2	intrinsic

1158. C₇H₈N₂O₄

Ethyl orotate

1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidine-carboxylic acid, ethyl ester

RN: 1747-53-1 MP (°C):

MW: 184.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-02	3.867E+00	20	N019	0 0 0 0 0	

1159. C₇H₈N₂S

1-Phenyl-2-thiourea

Phenylthioharnstoff

RN: 103-85-5 MP (°C): 149

MW: 152.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.708E-02	2.600E+00	18	F300	1 0 0 0 1	
3.830E-01	5.830E+01	100	F300	1 0 0 0 2	

1160. C₇H₈N₄O₂

Theophylline

1,3-Dimethylxanthine

Aerolate

Bronkotabs

Bronchodid Duracap

Bronkodyl

RN: 58-55-9**MP (°C):** 272**MW:** 180.17**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.310E-02	5.964E+00	16	A072	1 0 1 0 1	
2.866E-02	5.164E+00	20	K052	1 1 1 1 2	
1.380E+00	2.486E+02	25	B443	0 0 0 0 0	
3.420E-02	6.162E+00	25	F009	2 2 2 2 0	EFG
3.675E-02	6.621E+00	25	L338	1 0 1 1 2	
4.089E-02	7.366E+00	25	M128	2 0 1 2 2	
4.083E-02	7.356E+00	25	M158	2 0 2 2 2	
3.580E-02	6.450E+00	25	N312	2 1 1 1 1	
4.607E-02	8.300E+00	25	P010	1 0 1 1 1	
4.607E-02	8.300E+00	25	P011	0 0 0 0 0	
4.440E-02	8.000E+00	25	P018	1 0 2 2 1	
4.440E-02	8.000E+00	25	P020	2 0 1 1 1	
4.607E-02	8.300E+00	25	P312	0 0 0 0 0	
4.500E-02	8.108E+00	30	B042	1 2 1 1 1	
4.500E-02	8.108E+00	30	G021	1 0 0 0 2	
4.100E-02	7.387E+00	30	H016	2 2 2 2 0	EFG
4.500E-02	8.108E+00	30	H020	1 0 0 0 1	
5.550E-02	1.000E+01	37	F076	2 0 2 2 0	
2.761E-02	4.975E+00	ns	J025	0 0 0 0 2	
5.550E-03	1.000E+00	ns	K444	0 0 0 0 0	
3.580E-02	6.450E+00	ns	N062	2 0 1 2 2	
2.054E-04	3.700E-02	rt	N015	0 0 2 2 1	sic

1161. C₇H₈N₄O₂

Theobromine

Theobromin

RN: 83-67-0**MP (°C):** 357**MW:** 180.17**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.665E-03	3.000E-01	18	F300	1 0 0 0 0	
3.328E-03	5.996E-01	19	A072	1 0 1 0 0	
2.419E-03	4.358E-01	20	K052	1 1 1 1 2	
1.830E-03	3.297E-01	25	M158	2 0 2 2 2	
1.832E-03	3.300E-01	25	O302	1 0 0 1 0	
2.775E-03	5.000E-01	25	P010	1 0 1 1 1	
3.330E-03	6.000E-01	25	P011	0 0 0 0 0	
3.386E-03	6.100E-01	25	P018	1 0 2 2 1	

(continued)

1161. C₇H₈N₄O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.108E-03	5.600E-01	25	P020	2 0 1 1 1	
3.000E-03	5.405E-01	30	B042	1 2 1 1 0	
~3.00E-03	~5.41E-01	30	H020	1 0 0 0 0	
3.830E-02	6.900E+00	100	F300	1 0 0 0 1	
2.774E-03	4.998E-01	c	D004	0 0 0 0 0	
3.676E-02	6.623E+00	h	D004	0 0 0 0 0	
>2.77E-03	>5.00E-01	ns	B404	0 2 1 1 0	

1162. C₇H₈O*p*-Cresol

4-Cresol

p-Methylphenol

RN: 106-44-5

MP (°C): 35.5

MW: 108.14

BP (°C): 201.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.813E-01	1.961E+01	20	B031	1 0 2 2 1	
1.701E-01	1.840E+01	20	R087	0 0 0 0 0	0.15M NaCl
1.990E-01	2.152E+01	25	A021	1 2 1 1 0	
1.902E-01	2.057E+01	25	B019	1 0 1 2 0	
1.813E-01	1.961E+01	25	L022	1 0 0 0 0	
1.967E-01	2.127E+01	25	P004	0 0 0 0 0	
1.902E-01	2.057E+01	25	R041	0 0 0 0 0	
2.044E-01	2.210E+01	29.5	K119	1 0 0 0 2	
1.999E-01	2.162E+01	29.50	M098	1 2 0 1 2	
2.090E-01	2.260E+01	40	F300	1 0 0 0 2	
3.334E-01	3.605E+01	82.10	M098	1 2 0 1 2	

1163. C₇H₈O

Anisole

Methoxybenzene

Methyl phenyl ether

Phenyl methyl ether

RN: 100-66-3

MP (°C): -37.3

MW: 108.14

BP (°C): 155.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.295E-03	1.400E-01	25	A003	1 2 1 2 1	<i>sic</i>
9.609E-02	1.039E+01	25	B019	1 0 1 2 0	
1.000E-02	1.081E+00	25	D407	1 0 2 2 2	
1.400E-02	1.514E+00	25	M327	1 0 0 1 2	
1.418E-02	1.533E+00	25.04	V013	2 2 2 2 2	
9.617E-02	1.040E+01	26.70	L095	2 2 1 1 2	

1164. C₇H₈O

2-Cresol
 2-Methylphenol
 Phenol, 2-methyl-
o-Cresol
o-Methylphenol

RN: 95-48-7 **MP (°C):** 31
MW: 108.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.519E-01	2.724E+01	20	B031	1 0 2 2 1	
2.276E-01	2.461E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.312E-01	2.500E+01	23	P332	0 0 0 0 0	
2.400E-01	2.595E+01	25	A021	1 2 1 1 0	
1.991E-01	2.153E+01	25	B019	1 0 1 2 0	
2.127E-01	2.300E+01	25	B060	2 0 1 1 1	
2.400E-01	2.595E+01	25	B316	0 0 0 0 0	
2.300E-01	2.487E+01	25	F044	1 0 0 0 1	
2.423E-01	2.620E+01	25	F300	1 0 0 0 2	
2.569E-01	2.778E+01	25	L022	1 0 0 0 0	
2.999E-01	3.244E+01	25	P004	0 0 0 0 0	
2.255E-01	2.439E+01	25	R041	0 0 0 0 0	
1.991E-01	2.153E+01	31	B092	2 1 1 1 2	
2.606E-01	2.818E+01	46.20	M098	1 2 0 1 1	
2.497E-01	2.700E+01	50	K119	1 0 0 0 2	
2.763E-01	2.988E+01	60	B092	2 1 1 1 2	
3.557E-01	3.846E+01	86.70	M098	1 2 0 1 1	
2.291E-01	2.477E+01	ns	R427	0 0 0 0 0	

1165. C₇H₈O

m-Cresol
m-Cresol
m-Methylphenol

RN: 108-39-4 **MP (°C):** 11
MW: 108.14 **BP (°C):** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-01	1.147E+01	0	M041	1 1 0 0 2	
2.167E-01	2.344E+01	20	B031	1 2 2 2 1	
2.112E-01	2.284E+01	20	R087	0 0 0 0 0	0.15M NaCl
2.149E-01	2.324E+01	20.3	L339	2 0 2 2 2	
1.420E-01	1.536E+01	25	A021	1 2 1 1 0	
1.991E-01	2.153E+01	25	B019	1 0 1 2 0	
2.053E-01	2.220E+01	25	C060	1 2 1 1 2	
2.099E-01	2.270E+01	25	F300	1 0 0 0 2	
1.946E-01	2.105E+01	25	M041	1 1 0 0 2	
2.255E-01	2.439E+01	25	R041	0 0 0 0 0	
2.292E-01	2.478E+01	40.0	L339	2 0 2 2 2	

(continued)

1165. C₇H₈O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.682E-01	2.900E+01	46.2	K119	1 0 0 0 2	
2.326E-01	2.515E+01	50	M041	1 1 0 0 2	
2.431E-01	2.629E+01	50.80	M098	1 2 0 1 1	
2.712E-01	2.933E+01	58.4	L339	2 0 2 2 2	
2.693E-01	2.913E+01	60	B031	1 2 2 2 1	
3.331E-01	3.602E+01	77.2	L339	2 0 2 2 2	
3.213E-01	3.475E+01	78.70	M098	1 2 0 1 1	
3.982E-01	4.306E+01	92.20	M098	1 2 0 1 1	
4.387E-01	4.744E+01	98.1	L339	2 0 2 2 2	

1166. C₇H₈O

Benzyl alcohol

Benzylalkohol

Benzinemethanol

Phenylmethanol

Phenylcarbinol

α-Hydroxytoluene

RN: 100-51-6

MP (°C): -15.2

MW: 108.14

BP (°C): 204.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.606E-01	3.900E+01	17	F300	1 0 0 0 1	
3.488E-01	3.772E+01	20	H044	1 0 2 1 2	
3.520E-01	3.807E+01	20	S006	1 0 0 0 2	
3.967E-01	4.290E+01	25	B304	2 0 2 2 2	
3.540E-01	3.828E+01	25	H044	1 0 2 1 2	
4.260E-01	4.607E+01	25	L322	1 1 2 2 1	
3.616E-01	3.911E+01	30	H044	1 0 2 1 2	
3.646E-01	3.943E+01	35	H044	1 0 2 1 2	
3.676E-01	3.975E+01	40	H044	1 0 2 1 2	
3.724E-01	4.027E+01	45	H044	1 0 2 1 2	
3.722E-01	4.025E+01	50	H044	1 0 2 1 2	
3.868E-01	4.182E+01	55	H044	1 0 2 1 2	

1167. C₇H₈O₂

Salicyl alcohol

Salicylalkohol

RN: 90-01-7

MP (°C): 86

MW: 124.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.075E-01	6.300E+01	22	F300	1 0 0 0 1	

1168. C₇H₈O₂

Guaiacol

o-Methoxyphenol

RN: 90-05-1

MP (°C): 28

MW: 124.14

BP (°C): 205

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-01	1.870E+01	15	F300	1 0 0 0 2	
1.880E-01	2.334E+01	24.99	B353	0 0 0 0 0	
1.060E-02	1.316E+00	37	E028	1 0 1 1 2	
1.288E-03	1.599E-01	ns	R424	0 0 0 0 0	sic

1169. C₇H₈O₂

3-Methoxyphenol

Resorcinol monomethylether

p-Methoxyphenol

RN: 150-19-6

MP (°C):

MW: 124.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.110E-01	3.861E+01	25	B314	0 0 0 0 0	
3.110E-01	3.861E+01	30	B315	0 0 0 0 0	
4.000E-03	4.966E-01	37	E028	1 0 1 1 1	
4.966E-01	6.165E+01	ns	S460	0 0 0 0 0	sic

1170. C₇H₈O₂*p*-Methoxyphenol*p*-Hydroxyanisole

Hydroquinone monomethyl ether

4-Methoxyphenol

RN: 150-76-5

MP (°C): 52.5

MW: 124.14

BP (°C): 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.073E-01	2.573E+01	20	R087	0 0 0 0 0	0.15M NaCl

1171. C₇H₈O₂

4,6-Dimethyl-1,2-pyrone

4,6-Dimethyl- α -pyrone2,4-Dimethyl- α -pyrone

Mesitene lactone

4,6-Dimethyl-2-pyranone

4,6-Dimethyl-2H-pyran-2-one

RN: 675-09-2 **MP (°C):** 49**MW:** 124.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.953E+00	2.424E+02	59.7	W022	2 2 1 1 0	EFG
2.088E+00	2.593E+02	86.3	W022	2 2 1 1 0	EFG

1172. C₇H₈O₃S*p*-Toluenesulfonic acid

4-Methylbenzenesulfonic acid

Methylbenzenesulfonic acid

Tosic acid

PTSA

Toluene-4-sulfonic acid

RN: 104-15-4 **MP (°C):** 106.5**MW:** 172.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E+00	4.993E+02	36.5	T023	1 2 2 1 2	
2.902E+00	4.997E+02	40.5	T023	1 2 2 1 2	
2.903E+00	4.999E+02	42.5	T023	1 2 2 1 2	

1173. C₇H₈O₃S.H₂O*p*-Toluenesulfonic acid (monohydrate)**RN:** 6192-52-5 **MP (°C):** 104.5**MW:** 190.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.107E+00	4.008E+02	-6.5	T023	1 2 2 1 2	
2.120E+00	4.033E+02	-1.5	T023	1 2 2 1 2	
2.129E+00	4.050E+02	1.5	T023	1 2 2 1 2	
2.168E+00	4.125E+02	20.1	T023	1 2 2 1 2	
2.210E+00	4.203E+02	38.8	T023	1 2 2 1 2	
2.616E+00	4.975E+02	45.3	T023	1 2 2 1 2	
2.257E+00	4.293E+02	55.2	T023	1 2 2 1 2	
2.593E+00	4.933E+02	73.9	T023	1 2 2 1 2	
2.329E+00	4.431E+02	78.4	T023	1 2 2 1 2	
2.566E+00	4.882E+02	89.1	T023	1 2 2 1 2	
2.375E+00	4.517E+02	89.9	T023	1 2 2 1 2	

(continued)

1173. C₇H₈O₃S.H₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.446E+00	4.652E+02	101.1	T023	1 2 2 1 2	
2.525E+00	4.802E+02	102.9	T023	1 2 2 1 2	
2.498E+00	4.751E+02	104.8	T023	1 2 2 1 2	

1174. C₇H₈O₃S.2H₂O*o*-Toluenesulfonic acid (dihydrate)

RN: 68066-37-5 MP (°C):

MW: 208.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.718E+00	3.577E+02	-25.0	T023	1 2 2 1 2	
1.773E+00	3.691E+02	-13.0	T023	1 2 2 1 2	
1.823E+00	3.795E+02	.8	T023	1 2 2 1 2	
1.891E+00	3.938E+02	16.8	T023	1 2 2 1 2	
1.954E+00	4.068E+02	31.2	T023	1 2 2 1 2	
2.264E+00	4.715E+02	48.2	T023	1 2 2 1 2	
2.055E+00	4.279E+02	50.0	T023	1 2 2 1 2	
2.243E+00	4.671E+02	54.0	T023	1 2 2 1 2	
2.090E+00	4.353E+02	56.0	T023	1 2 2 1 2	
2.207E+00	4.597E+02	60.4	T023	1 2 2 1 2	
2.148E+00	4.472E+02	61.2	T023	1 2 2 1 2	
2.179E+00	4.538E+02	62.0	T023	1 2 2 1 2	

1175. C₇H₈O₃S.4H₂O*p*-Toluenesulfonic acid (tetrahydrate)

RN: 104-15-4 MP (°C):

MW: 244.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.422E+00	3.473E+02	-27.0	T023	1 2 2 1 2	
1.437E+00	3.510E+02	-26.0	T023	1 2 2 1 2	
1.450E+00	3.543E+02	-18.5	T023	1 2 2 1 2	
1.527E+00	3.730E+02	-16.5	T023	1 2 2 1 2	
1.592E+00	3.888E+02	-10.5	T023	1 2 2 1 2	
1.613E+00	3.939E+02	-8.5	T023	1 2 2 1 2	
1.640E+00	4.005E+02	-7.0	T023	1 2 2 1 2	
1.576E+00	3.848E+02	-5.9	T023	1 2 2 1 2	
1.605E+00	3.921E+02	-3.4	T023	1 2 2 1 2	
1.622E+00	3.961E+02	-2.2	T023	1 2 2 1 2	
1.641E+00	4.008E+02	-1.0	T023	1 2 2 1 2	

1176. C₇H₈O₇

Methylenecitric acid

Methylen-citronensaeure

RN: 144-16-1 **MP (°C):**
MW: 204.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.337E-01	4.770E+01	20	F300	1 0 0 0 2	

1177. C₇H₉ClN₂OS

TO-2

5-Chloro-4-methyl-2-propionamide-thiazole

CMPT

RN: 13915-79-2 **MP (°C):** 159
MW: 204.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.794E-04	1.800E-01	ns	M061	0 0 0 0 2	

1178. C₇H₉N

4-Ethylpyridine

4-Aethyl-pyridin

RN: 536-75-4 **MP (°C):** -90.5
MW: 107.16 **BP (°C):** 168.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.906E+00	4.186E+02	-19	C047	2 2 0 0 1	
2.495E+00	2.674E+02	182	C047	2 2 0 0 2	

1179. C₇H₉N

m-Toluidine

3-Toluidine

4-Methylaniline

p-Toluidine

p-Toluidin

RN: 106-49-0 **MP (°C):** 43
MW: 107.16 **BP (°C):** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.066E-02	6.500E+00	15	F300	1 0 0 0 1	
6.026E-02	6.457E+00	20	B179	0 0 0 0 0	
3.890E-01	4.169E+01	20	B179	0 0 0 0 0	
1.403E-01	1.503E+01	20	C113	1 0 2 1 2	
6.200E-02	6.644E+00	20	H306	1 0 1 2 1	
6.119E-02	6.557E+00	20	T301	1 2 2 2 2	

1180. C₇H₉N

Methylaniline

N-Methylaniline

RN: 100-61-8 **MP (°C):** -57
MW: 107.16 **BP (°C):** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.248E-02	5.624E+00	25	C113	1 0 2 1 2	

1181. C₇H₉N

3,4-Lutidine

3,4-Dimethylpyridine

RN: 583-58-4 **MP (°C):** -12
MW: 107.16 **BP (°C):** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E+00	1.968E+02	-3.6	C047	2 2 0 0 2	
2.470E+00	2.647E+02	163	C047	2 2 0 0 1	
+2.29E+00	+2.45E+02	ns	S460	0 0 0 0 0	

1182. C₇H₉N*o*-Toluidine

2-Toluidine

RN: 95-53-4 **MP (°C):** -15
MW: 107.16 **BP (°C):** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.524E-01	1.633E+01	20	C113	1 0 2 1 2	
1.577E-01	1.690E+01	20	K119	1 0 0 0 2	
1.381E-01	1.480E+01	25	F300	1 0 0 0 2	

1183. C₇H₉N

3-Ethylpyridine

3-Aethyl-pyridin

 β -Lutidine

RN: 536-78-7 **MP (°C):**
MW: 107.16 **BP (°C):** 163

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.520E+00	2.701E+02	196	C047	2 2 0 0 1	

1184. C₇H₉N

3,5-Lutidine

3,5-Dimethylpyridine

RN: 591-22-0 **MP (°C):** -9
MW: 107.16 **BP (°C):** 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E+00	2.032E+02	-12	C047	2 2 0 0 2	
2.520E+00	2.701E+02	192	C047	2 2 0 0 1	
+2.40E+00	+2.57E+02	ns	S460	0 0 0 0 0	

1185. C₇H₉N

2,6-Lutidine

2,6-Dimethyl-pyridin

2,6-Dimethylpyridine

RN: 108-48-5 **MP (°C):** -6
MW: 107.16 **BP (°C):** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.154E+00	2.308E+02	34	C047	2 2 0 0 1	
2.714E+00	2.908E+02	231	C047	2 2 0 0 1	
+2.82E+00	+3.02E+02	ns	S460	0 0 0 0 0	

1186. C₇H₉N

2,5-Lutidine

2,5-Dimethyl-pyridin

2,5-Dimethylpyridine

RN: 589-93-5 **MP (°C):** -15
MW: 107.16 **BP (°C):** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.984E+00	2.126E+02	13.1	C047	2 2 0 0 1	
7.186E-01	7.700E+01	23	F300	1 0 0 0 1	
2.570E+00	2.754E+02	207	C047	2 2 0 0 1	

1187. C₇H₉N

2,4-Lutidine

2,4-Dimethyl-pyridin

2,4-Dimethylpyridine

RN: 108-47-4 **MP (°C):** -60
MW: 107.16 **BP (°C):** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.961E+00	4.245E+02	23	J007	1 2 0 1 2	average of 2
1.896E+00	2.032E+02	23.4	C047	2 2 0 0 2	

(continued)

1187. C₇H₉N (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E+00	2.032E+02	23.40	A009	1 2 1 1 2	LCST
1.287E+00	1.379E+02	24.40	A009	1 2 1 1 2	EFG, LCST
2.419E+00	2.593E+02	25	A009	1 2 1 1 2	EFG, LCST
3.316E+00	3.553E+02	27.2	J007	1 2 0 1 2	
8.484E-01	9.091E+01	30	A009	1 2 1 1 2	EFG, LCST
3.111E+00	3.333E+02	32.50	A009	1 2 1 1 2	EFG, LCST
4.497E+00	4.819E+02	35.0	J007	1 2 0 1 2	
2.902E+00	3.110E+02	39.0	J007	1 2 0 1 2	
6.105E-01	6.542E+01	40	A009	1 2 1 1 2	EFG, LCST
3.500E+00	3.750E+02	50	A009	1 2 1 1 2	EFG, LCST
2.545E+00	2.727E+02	53	J007	1 2 0 1 2	
4.548E+00	4.873E+02	54.3	J007	1 2 0 1 2	
3.777E+00	4.048E+02	62.50	A009	1 2 1 1 2	EFG, LCST
2.204E+00	2.362E+02	68.5	J007	1 2 0 1 2	
6.105E-01	6.542E+01	149	A009	1 2 1 1 2	EFG, UCST
3.794E+00	4.065E+02	165	A009	1 2 1 1 2	EFG, UCST
1.287E+00	1.379E+02	180	A009	1 2 1 1 2	EFG, UCST
3.500E+00	3.750E+02	180	A009	1 2 1 1 2	EFG, UCST
3.111E+00	3.333E+02	186	A009	1 2 1 1 2	EFG, UCST
1.896E+00	2.032E+02	187	A009	1 2 1 1 2	EFG, UCST
2.419E+00	2.593E+02	187	A009	1 2 1 1 2	EFG, UCST
2.520E+00	2.701E+02	189	A009	1 2 1 1 2	
2.520E+00	2.701E+02	189	C047	2 2 0 0 1	UCST

1188. C₇H₉N

2,3-Lutidine

2,3-Dimethylpyridine

RN: 583-61-9 **MP (°C):** -15
MW: 107.16 **BP (°C):** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.926E+00	2.063E+02	16.5	C047	2 2 0 0 1	
2.594E+00	2.780E+02	193	C047	2 2 0 0 2	
+2.40E+00	+2.57E+02	ns	S460	0 0 0 0 0	

1189. C₇H₉N

2-Ethylpyridine

α-Lutidine

RN: 100-71-0 **MP (°C):**
MW: 107.16 **BP (°C):** 149

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.368E+00	2.537E+02	-5	C047	2 2 0 0 1	
2.760E+00	2.958E+02	231	C047	2 2 0 0 1	
+3.24E+00	+3.47E+02	ns	S460	0 0 0 0 0	

1190. C₇H₉NO*p*-Anisidine

4-Methoxybenzenamine

p-Methoxyaniline

4-Methoxy-1-aminobenzene

p-Methoxyphenylamine

RN: 104-94-9 **MP (°C):** 57
MW: 123.16 **BP (°C):** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.311E-02	1.147E+01	20	T301	1 2 2 2 2	

1191. C₇H₉NO*p*-Tolylhydroxylamine*p*-Tolylhydroxylamin

RN: 623-10-9 **MP (°C):**
MW: 123.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.120E-02	1.000E+01	5	F300	1 0 0 0 1	
4.027E-01	4.960E+01	100	F300	1 0 0 0 2	

1192. C₇H₉NO*o*-Anisidine

2-Anisidine

2-Methoxybenzenamine

o-Methoxyaniline

2-Methoxy-1-aminobenzene

o-Methoxyphenylamine

RN: 90-04-0 **MP (°C):** 5
MW: 123.16 **BP (°C):** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-01	1.264E+01	25	B019	1 0 1 2 0	

1193. C₇H₉NO₂

1,2-Dimethyl-3-hydroxy-4-pyridone

DMHP

RN: 30652-11-0 **MP (°C):** 271–273
MW: 139.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-01	1.572E+01	25	C340	0 0 0 0 0	pH 9.4

1194. C₇H₉NO₂S*p*-Toluenesulfonamide*p*-Methylbenzenesulfonamide

4-Methylbenzenesulfonamide

RN: 70-55-3 MP (°C): 138

MW: 171.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	1.900E+00	9	F300	1 0 0 0 1	
1.180E-02	2.020E+00	15	K024	1 2 1 1 2	
1.843E-02	3.156E+00	25	H105	1 1 0 1 2	

1195. C₇H₉NO₂S*o*-Toluenesulfonamide*o*-Methylbenzenesulfonamide

RN: 88-19-7 MP (°C): 156

MW: 171.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.840E-03	1.000E+00	9	F300	1 0 0 0 0	
1.860E-02	3.185E+00	15	K024	1 2 1 1 2	
9.485E-03	1.624E+00	25	H105	1 1 0 1 2	

1196. C₇H₉NO₂S*m*-Toluenesulfonamide*m*-Methylbenzenesulfonamide

RN: 1899-94-1 MP (°C):

MW: 171.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.750E-02	2.996E+00	15	K024	1 2 1 1 2	
4.563E-02	7.812E+00	25	H105	1 1 0 1 2	

1197. C₇H₉NO₃S

4-Amino-3-methylbenzene sulfonic acid

4-Amino-toluol-sulfosaeure-(3)

RN: 98-33-9 MP (°C):

MW: 187.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.671E-02	5.000E+00	20	F300	1 0 0 0 0	

1198. C₇H₉NO₃S

4-Amino-2-methylbenzene sulfonic acid

4-Amino-toluol-sulfosaeure-(2)

RN: 133-78-8 **MP (°C):****MW:** 187.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.404E-02	4.500E+00	20	F300	1 0 0 0 1	

1199. C₇H₉NO₃S

2-Amino-5-methylbenzene sulfonic acid

2-Amino-toluol-sulfosaeure-(5)

RN: 88-44-8 **MP (°C):** >300**MW:** 187.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-01	3.200E+01	19	F300	1 0 0 0 1	

1200. C₇H₉NO₃S*p*-Methoxybenzenesulfonamide

4-Methoxybenzenesulfonamide

RN: 1129-26-6 **MP (°C):****MW:** 187.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-02	2.921E+00	15	K024	1 2 1 1 2	

1201. C₇H₉N₃O

4-Phenylsemicarbazide

Phenylsemicarbazide

RN: 537-47-3 **MP (°C):** 123.5**MW:** 151.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.995E-01	15	D068		1 2 0 0 0	

1202. C₇H₉N₃O₂S₂

Sulfathiourea

p-Aminobenzenesulfonylthiourea*p*-Aminophenylsulfonylthiourea

Badional

Baldinol

Fontamide

RN: 515-49-1 **MP (°C):** 171.5**MW:** 231.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.365E-03	5.470E-01	20	F073	1 2 2 2 2	

1203. C₇H₉N₃O₃

Orotic acid ethylamide

RN: 1011-82-1 **MP (°C):** 263–265**MW:** 183.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-01	3.553E+01	–4	N018	0 0 0 0 0	
3.240E-01	5.935E+01	16	N018	0 0 0 0 0	
3.980E-01	7.290E+01	25	N018	0 0 0 0 0	

1204. C₇H₉N₃O₃S

Sulfanilylurea

Sulfanilylharnstoff

RN: 547-44-4 **MP (°C):** 146**MW:** 215.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	2.333E+00	20	F073	1 2 2 2 2	
5.575E-03	1.200E+00	37	F300	1 0 0 0 1	
5.012E-02	1.079E+01	ns	R427	0 0 0 0 0	

1205. C₇H₉N₃O₄

Orotic acid ethanol amide

RN: **MP (°C):** 217–218**MW:** 199.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-01	3.585E+01	–4	N018	0 0 0 0 0	
3.460E-01	6.891E+01	16	N018	0 0 0 0 0	
4.470E-01	8.903E+01	25	N018	0 0 0 0 0	

1206. C₇H₉O₃P

Hydroxymethylphenylphosphinic acid

RN: 61451-78-3 **MP (°C):** 138
MW: 172.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.166E+02	2.007E+04	0	W422	0 0 0 0 0	
9.900E+00	1.704E+03	34.29	W422	0 0 0 0 0	
2.060E+01	3.546E+03	44.30	W422	0 0 0 0 0	
4.240E+01	7.298E+03	54.41	W422	0 0 0 0 0	
9.660E+01	1.663E+04	64.99	W422	0 0 0 0 0	
1.662E+02	2.861E+04	73.42	W422	0 0 0 0 0	
2.474E+02	4.258E+04	79.6	W422	0 0 0 0 0	
3.120E+02	5.370E+04	83.95	W422	0 0 0 0 0	

1207. C₇H₁₀

1,3-Cycloheptadiene

RN: 4054-38-0 **MP (°C):**
MW: 94.16 **BP (°C):** 121

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.577E-03	6.192E-01	ns	S460	0 0 0 0 0	

1208. C₇H₁₀N₂OS

Propylthiouracil

6-Propyl-2-thiouracil

Propycil

RN: 51-52-5 **MP (°C):** 220.0
MW: 170.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.520E-03	1.110E+00	20	A091	1 0 0 0 0	
6.455E-03	1.099E+00	20	I310	0 0 0 0 0	
7.070E-03	1.204E+00	25	G016	1 2 1 2 2	intrinsic
5.816E-02	9.901E+00	100	I310	0 0 0 0 0	
5.874E-03	1.000E+00	ns	K444	0 0 0 0 0	

1209. C₇H₁₀N₂O₂S

p-Methylaminobenzenesulfonamide

4-Methylaminobenzenesulfonamide

RN: 16891-79-5 **MP (°C):**
MW: 186.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	9.312E-01	15	K024	1 2 1 1 2	

1210. C₇H₁₀N₂O₂S

N1-Methylsulfanilamide

4-Amino-*N*-methylbenzenesulfonamide*N*-Methyl-*p*-aminobenzenesulfonamide*N*-Methyl-4-aminobenzenesulfonamide**RN:** 1709-52-0 **MP (°C):****MW:** 186.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.450E-02	1.760E+01	37	K095	2 0 0 0 2	intrinsic

1211. C₇H₁₀N₂O₂S

Toluenesulfamide

Sulfamide, (4-methylphenyl)-

p-Tolylsulfamide**RN:** 15853-38-0 **MP (°C):****MW:** 186.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-02	5.624E+00	37	A028	1 0 2 1 2	intrinsic

1212. C₇H₁₀N₂O₃

Isopropylbarbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1-methylethyl)-

Isopropylbarbiturate

RN: 7391-69-7 **MP (°C):****MW:** 170.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.482E-02	5.925E+00	20	J030	1 2 2 2 2	
5.905E-02	1.005E+01	37	J030	1 2 2 2 2	

1213. C₇H₁₀N₂O₃

5-Ethyl-5-methylbarbituric acid

5-Methyl-5-ethylbarbituric acid

RN: 27653-63-0 **MP (°C):****MW:** 170.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.010E-02	1.363E+01	25	M310	2 2 2 2 2	
5.912E-02	1.006E+01	25	P350	0 0 0 0 0	intrinsic

1214. C₇H₁₀N₄O₂S

Sulfanilylguanidine

Sulfaguanidine

Sulfaguanidin

Sulfanilguanidin

RN: 57-67-0**MP (°C):** 190**MW:** 214.25**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.131E-03	8.850E-01	20	F073	1 2 2 2 2	
4.663E-03	9.990E-01	25	D041	1 0 0 0 0	
8.868E-03	1.900E+00	37	R045	1 2 1 1 2	
1.025E-02	2.195E+00	37.50	M142	1 2 0 0 2	
4.201E-01	9.000E+01	h	F300	0 0 0 0 0	

1215. C₇H₁₀N₄O₃.H₂O

Theopylline (monohydrate)

1H-Purine-2,6-dione, 3,7-dihydro-1,3-dimethyl-, monohydrate

RN: 5967-84-0**MP (°C):** 269–272**MW:** 216.20**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.823E-02	8.264E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

1216. C₇H₁₀O₄S.H₂O

o-Toluenesulfonic acid (monohydrate)

2-Methyl-benzenesulfonic acid (monohydrate)

RN: 88-20-0**MP (°C):****MW:** 208.23**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E+00	4.889E+02	32.5	T023	1 2 2 1 2	
2.335E+00	4.863E+02	38.6	T023	1 2 2 1 2	
2.318E+00	4.827E+02	45.7	T023	1 2 2 1 2	
2.266E+00	4.718E+02	48.5	T023	1 2 2 1 2	
2.302E+00	4.793E+02	48.6	T023	1 2 2 1 2	
2.273E+00	4.733E+02	49.0	T023	1 2 2 1 2	
2.289E+00	4.767E+02	49.6	T023	1 2 2 1 2	

1217. C₇H₁₀O₅

Shikimic acid

Shikimisaeure

RN: 138-59-0 **MP (°C):** 190
MW: 174.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.613E-01	1.500E+02	21	F300	1 0 0 0 1	

1218. C₇H₁₀O₅

Mesoxalic acid diethyl ester

Mesooxalsaeure-diaethyl ester

RN: 609-09-6 **MP (°C):** -30
MW: 174.15 **BP (°C):** 208

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.249E+00	5.658E+02	22	F300	1 0 0 0 2	
+3.25E+00	+5.66E+02	ns	S460	0 0 0 0 0	

1219. C₇H₁₁NO₂

Ethosuximide

Zarontin

2-Ethyl-2-methylsuccinimide

RN: 77-67-8 **MP (°C):**
MW: 141.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.346E+00	1.900E+02	25	P061	0 0 0 0 0	pH 3-7.9
7.084E-01	1.000E+02	ns	K444	0 0 0 0 0	

1220. C₇H₁₁N₃O₂

Ipronidazole

1-Methyl-2-isopropyl-5-nitro-imidazole

RN: 14885-29-1 **MP (°C):** 58–60
MW: 169.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.556E-02	9.400E+00	20	D344	0 0 0 0 0	
5.550E-02	9.390E+00	20	D344	0 0 0 0 0	
5.446E-02	9.214E+00	20	D344	0 0 0 0 0	
5.560E-02	9.407E+00	20	D344	0 0 0 0 0	

1221. C₇H₁₁N₃O₂

1-Methyl-L-histidine

L-1-Methylhistidine

RN: 15507-76-3 MP (°C): >254

MW: 169.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.851E-01	1.667E+02	25	D041	1 0 0 0 0	

1222. C₇H₁₁N₇S

Aziprotryne

2-Azido-4-isopropylamino-6-methylmercapto-s-triazine

C-7019

RN: 4658-28-0 MP (°C): 95

MW: 225.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.441E-04	5.500E-02	20	M161	1 0 0 0 1	
3.329E-04	7.500E-02	ns	M061	0 0 0 0 1	

1223. C₇H₁₂

1,6-Heptadiene

RN: 3070-53-9 MP (°C): -129.0

MW: 96.17 BP (°C): 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.575E-04	4.400E-02	25	M001	2 1 2 2 1	

1224. C₇H₁₂

1-Heptyne

1-*n*-Heptyne

Pentylacetylene

Amylacetylene

RN: 628-71-7 MP (°C): -81

MW: 96.17 BP (°C): 99

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.774E-04	9.400E-02	25	M001	2 1 2 2 2	

1225. C₇H₁₂

Cycloheptene
(1Z)-Cycloheptene
cis-Cycloheptene

RN: 628-92-2 **MP (°C):** -56
MW: 96.17 **BP (°C):** 114.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.863E-04	6.600E-02	25	M001	2 1 2 2 1	

1226. C₇H₁₂

1-Methyl-1-cyclohexene
1-Methylcyclohexene

RN: 591-49-1 **MP (°C):** -120
MW: 96.17 **BP (°C):** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.407E-04	5.200E-02	25	M001	2 1 2 2 2	

1227. C₇H₁₂

2-Heptyne
1-Methyl-2-butylacetylene
Butyl(methyl)acetylene

RN: 1119-65-9 **MP (°C):**
MW: 96.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	1.635E-01	25	H039	1 2 2 2 2	

1228. C₇H₁₂

2-Methyl-3-hexyne
1-Ethyl-2-isopropylacetylene

RN: 36566-80-0 **MP (°C):**
MW: 96.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	1.731E-01	25	H039	1 2 2 2 2	

1229. C₇H₁₂BrNO₄

5-Bromo-2-propyl-5-nitro-1,3-dioxane

2-Propyl-5-bromo-5-nitro-1,3-dioxane

RN: 53983-01-0 MP (°C): 73–75

MW: 254.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.102E-03	2.799E-01	25	L013	1 0 2 1 2	

1230. C₇H₁₂ClN₅

Norazine

2-Chloro-4-methylamino-6-isopropylamino-s-triazine

RN: 3004-71-5 MP (°C): 157–159

MW: 201.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-03	2.600E-01	20	J033	0 0 0 0 0	
1.289E-03	2.600E-01	21	B192	0 0 0 0 2	

1231. C₇H₁₂ClN₅

Simazine

2-Chloro-4-ethylamino-6-ethylamino-s-triazine

2-Chloro-4,6-bis(ethylamino)-s-triazine

Primatol S

RN: 122-34-9 MP (°C): 224

MW: 201.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.918E-06	2.000E-03	10	B185	0 0 0 0 0	
2.512E-05	5.065E-03	20	B179	0 0 0 0 0	
2.479E-05	5.000E-03	20	B185	0 0 0 0 0	
2.827E-05	5.700E-03	20	C048	2 2 2 2 1	
1.736E-05	3.500E-03	20	F311	1 2 2 2 1	
2.479E-05	5.000E-03	21	B192	0 0 0 0 0	
2.479E-05	5.000E-03	21	G099	2 0 0 1 0	
2.479E-05	5.000E-03	22	M061	1 0 0 0 0	
7.500E-05	1.512E-02	26	G001	1 0 1 1 1	
1.310E-04	2.642E-02	50	G001	1 0 1 1 2	
4.165E-04	8.400E-02	85	B185	0 0 0 0 0	
4.110E-04	8.288E-02	85	B200	1 0 0 0 2	
1.736E-05	3.500E-03	ns	C101	0 0 0 0 1	
2.479E-05	5.000E-03	ns	G041	0 0 0 0 0	
2.479E-05	5.000E-03	ns	H112	0 0 0 0 0	
2.479E-05	5.000E-03	ns	J033	0 0 0 0 0	
3.074E-05	6.200E-03	ns	V414	0 0 0 0 0	
2.479E-05	5.000E-03	rt	M161	0 0 0 0 0	

1232. C₇H₁₂ClN₅

2-Chloro-4-methyl amino-6-propyl amino-*s*-triazine
 1,3,5-Triazine-2,4-diamine, 6-chloro-*N*-methyl-*N'*-propyl-
s-Triazine, 2-chloro-4-methylamino-6-propylamino-

RN: 73383-40-1 **MP (°C):**

MW: 201.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.289E-03	2.600E-01	21	G099	2 0 0 1 0	

1233. C₇H₁₂N₂O₂

5-Isobutylhydantoin

Hydantoin of DL-leucine

RN: 67337-73-9 **MP (°C):** 208

MW: 156.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-02	1.937E+00	ns	M025	0 2 0 1 2	

1234. C₇H₁₂N₄O₅

Diglycine hydantoic acid

Carbamidoglycylglycine

RN: **MP (°C):** 194

MW: 232.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.260E-01	2.926E+01	25	M024	1 2 0 1 2	

1235. C₇H₁₂N₄O₅

Carbamidodiglycylglycine

Triglycine hydantoin acid

RN: **MP (°C):** 204

MW: 232.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.460E-02	1.036E+01	25	M024	1 2 0 1 2	

1236. C₇H₁₂O

3-Methylcyclohexanone

m-Methylcyclohexanone

RN: 591-24-2 **MP (°C):** -75
MW: 112.17 **BP (°C):** 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.335E-02	1.498E+00	20	D052	1 1 0 0 0	
1.349E-02	1.513E+00	ns	S460	0 0 0 0 0	

1237. C₇H₁₂O

2-Methylcyclohexanone

Methyl anone

o-Methylcyohexanone

Methyl cyclohexanone

RN: 583-60-8 **MP (°C):**
MW: 112.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-01	1.274E+01	23.50	O005	2 0 2 2 2	

1238. C₇H₁₂O₂

Hexahydrobenzoic acid

Cyclohexanecarboxylic acid

Cyclohexan-carbonsaeure

RN: 98-89-5 **MP (°C):** 31
MW: 128.17 **BP (°C):** 232.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	2.006E+00	15	L006	1 0 0 0 2	
1.560E-02	2.000E+00	21	F300	1 0 0 0 0	

1239. C₇H₁₂O₂

Isobutyl propenoate

2-methylpropyl acrylate

2-Propenoic acid, 2-methylpropyl ester

Acrylic acid isobutyl ester

Isobutyl 2-propenoate

Isobutyl acrylate

RN: 106-63-8 **MP (°C):**
MW: 128.17 **BP (°C):** 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.166E-02	7.903E+00	ns	S460	0 0 0 0 0	

1240. C₇H₁₂O₄

Pimelic acid

Heptanedioic acid

RN: 111-16-0

MP (°C): 105.7

MW: 160.17

BP (°C): 272

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.115E-01	1.786E+01	5.99	A341	0 0 0 0 0	
1.151E-01	1.844E+01	7.99	A341	0 0 0 0 0	
1.334E-01	2.137E+01	10.99	A341	0 0 0 0 0	
1.523E-01	2.439E+01	13	D041	1 0 0 0 1	
1.498E-01	2.400E+01	13.50	F300	1 0 0 0 1	
3.122E-01	5.000E+01	15	M051	1 0 0 0 1	
2.236E-01	3.582E+01	15.99	A341	0 0 0 0 0	
2.527E-01	4.048E+01	17.99	A341	0 0 0 0 0	
3.006E-01	4.815E+01	19.99	A341	0 0 0 0 0	
2.973E-01	4.762E+01	20	D041	1 0 0 0 0	
3.122E-01	5.000E+01	20	L041	1 0 0 1 1	
2.953E-01	4.730E+01	20	M171	1 0 0 0 1	
3.000E-02	4.805E+00	20	S006	1 0 0 0 1	
3.332E+00	5.337E+02	21	B040	1 0 1 1 2	sic
3.846E-01	6.160E+01	23.99	A341	0 0 0 0 0	
3.938E-01	6.307E+01	24.99	A341	0 0 0 0 0	
4.660E-01	7.464E+01	28.99	A341	0 0 0 0 0	
5.072E-01	8.124E+01	30.99	A341	0 0 0 0 0	
5.690E-01	9.114E+01	33.99	A341	0 0 0 0 0	
6.545E-01	1.048E+02	36.99	A341	0 0 0 0 0	
8.886E-01	1.423E+02	39.99	A341	0 0 0 0 0	
1.527E+00	2.446E+02	42.99	A341	0 0 0 0 0	
1.824E+00	2.922E+02	44.99	A341	0 0 0 0 0	
2.135E+00	3.420E+02	47.49	A341	0 0 0 0 0	
2.551E+00	4.086E+02	49.99	A341	0 0 0 0 0	
3.460E+00	5.542E+02	54.82	A341	0 0 0 0 0	
3.915E+00	6.270E+02	59.99	A341	0 0 0 0 0	
4.365E+00	6.991E+02	64.49	A341	0 0 0 0 0	
4.649E+00	7.446E+02	68.99	A341	0 0 0 0 0	
3.937E-01	6.306E+01	rt	H431	0 0 0 0 0	

1241. C₇H₁₂O₄

Diethyl malonate

Malonic

Malonic ester

Propanedioic acid diethyl ester

Ethyl propanedioate

Ethyl methane dicarboxylate

RN: 105-53-3 **MP (°C):** -50**MW:** 160.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.851E+00	6.169E+02	25	H430	0 0 0 0 0	
1.450E-01	2.322E+01	37	E028	1 0 1 1 2	

1242. C₇H₁₂O₄Ethyl α -acetoxypropionate

Ethyl 2-(acetoxy)propanoate

Ethyl 2-acetoxypropionate

RN: 2985-28-6 **MP (°C):****MW:** 160.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.104E-01	3.370E+01	25	R006	2 2 0 1 2	

1243. C₇H₁₂O₄

3-Methyladipic acid

3-Methylhexanedioic acid

RN: 3058-01-3 **MP (°C):** 101**MW:** 160.17 **BP (°C):** 230

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.986E-01	6.385E+01	9.50	A031	1 2 2 2 2	
4.732E-01	7.579E+01	12.80	A031	1 2 2 2 2	
1.241E+00	1.987E+02	25.90	A031	1 2 2 2 2	
1.865E+00	2.987E+02	29.80	A031	1 2 2 2 2	
2.531E+00	4.055E+02	33.20	A031	1 2 2 2 2	
3.707E+00	5.938E+02	41.10	A031	1 2 2 2 2	
4.663E+00	7.468E+02	52.30	A031	1 2 2 2 2	
5.340E+00	8.553E+02	64.30	A031	1 2 2 2 2	

1244. C₇H₁₂O₄*n*-Butylmalonic acidAcide *n*-butylmalonique

RN: 534-59-8 MP (°C): 102
 MW: 160.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.242E-01	1.160E+02	0	M051	1 0 0 0 2	
1.898E+00	3.040E+02	15	M051	1 0 0 0 2	
2.735E+00	4.380E+02	25	M051	1 0 0 0 2	
4.951E+00	7.930E+02	50	M051	1 0 0 0 2	

1245. C₇H₁₂O₅

Propanoic acid, 2-[(ethoxycarbonyl)oxy]-, methyl ester

RN: MP (°C):
 MW: 176.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.214E-02	1.623E+01	25	R007	0 0 0 0 0	

1246. C₇H₁₂O₆

Quinic acid

Chinasaeure

D-(*–*)-Quinic acid

1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid

RN: 77-95-2 MP (°C): 162
 MW: 192.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.509E+00	2.900E+02	9	F300	1 0 0 0 1	

1247. C₇H₁₃BrN₂O₂

Carbromal

Adalin

Bromodiethylacetylurea

N-(Aminocarbonyl)-2-bromo-2-ethylbutanamide

1-Bromo-ethyl-butylurea

Bromodiethylacetylcarbamide

RN: 77-65-6 MP (°C): 117
 MW: 237.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.109E-03	5.000E-01	20	F300	1 0 0 0 0	

1248. C₇H₁₃BrN₂O₂

Bromo-pivalate ureide

RN: MP (°C):
MW: 237.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.161E-01	5.123E+01	ns	F057	0 2 2 2 1	

1249. C₇H₁₃NO₂S

2-Ethyl-2-methyl-4-thiazolidinecarboxylic acid
 4-Thiazolidinecarboxylic acid, 2-ethyl-2-methyl-
 Thiazolidine-4-carboxylic acid, 2-ethyl-2-methyl-

RN: 56595-20-1 **MP (°C):**
MW: 175.25 **BP (°C):** 327.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-01	4.557E+01	21	B414	1 0 0 1 1	very fast and extent decomposition, uncertain value

1250. C₇H₁₃NO₂S

2-Propylthiazolidine-4-carboxylic acid
 4-Thiazolidinecarboxylic acid, 2-propyl-

RN: 4165-34-8 **MP (°C):**
MW: 175.25 **BP (°C):** 346.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-02	1.490E+01	21	B414	1 0 0 1 1	partial decomposition

1251. C₇H₁₃NO₂S₂

2,2-(Dimethyl)-4-(methoxycarbamyl)-1,3-dithiolane
 1,3-Dithiolane-4-methanol, 2,2-dimethyl-, carbamate

RN: 35801-62-8 **MP (°C):**
MW: 207.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	1.244E+00	rt	B174	0 0 1 0 0	

1252. C₇H₁₃NO₃

N-Formylleucine

N-Formyl-DL-leucine

RN: 6113-61-7

MP (°C):

MW: 159.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-01	2.945E+01	ns	M025	0 2 0 1 2	

1253. C₇H₁₃NO₃S

2,2-(Dimethyl)-4-(methoxycarbamyl)-1,3-oxathiolane

1,3-Oxathiolane-5-methanol, 2,2-dimethyl-, carbamate

RN: 78002-88-7 MP (°C):

MW: 191.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	5.738E+00	rt	B174	0 0 1 0 0	

1254. C₇H₁₃N₃O₃S

Oxamyl

Vydate

Thioxamyl

N,N'-Dimethyl-N-[(methylcarbamoyl)oxy]-1-thiooxamimidic acid methyl ester

N,N-Dimethyl- α -methylcarbamoyloxyimino- α -(methylthio)acetamide

DPX 1410

RN: 23135-22-0 MP (°C): 109

MW: 219.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.288E+00	2.825E+02	20	B179	0 0 0 0 0	
1.277E+00	2.800E+02	25	M161	1 0 0 0 2	
9.977E-01	2.188E+02	ns	H308	0 0 0 0 1	

1255. C₇H₁₃N₅O

Hydroxysimazine

1,3,5-Triazin-2(1H)-one, 4,6-bis(ethylamino)-

2-Hydroxysimazine

4,6-bis(Ethylamino)-s-triazin-2-ol

G 30414

RN: 2599-11-3 MP (°C):

MW: 183.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	2.748E-02	2	B193	1 1 0 0 1	

1256. C₇H₁₄

1-Heptene

1-*n*-Heptene*n*-Hept-1-ene**RN:** 592-76-7**MP (°C):** -119**MW:** 98.19**BP (°C):** 93.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	1.817E-02	25	M342	1 0 1 1 2	

1257. C₇H₁₄

2-Heptene

RN: 592-77-8**MP (°C):****MW:** 98.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-04	1.500E-02	23.5	S171	2 1 2 2 2	
1.528E-04	1.500E-02	25	M001	2 1 2 2 1	

1258. C₇H₁₄

Cycloheptane

RN: 291-64-5**MP (°C):** -12**MW:** 98.19**BP (°C):** 118.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-04	1.820E-02	20	M337	2 1 2 2 2	
3.055E-04	3.000E-02	25	M001	2 1 2 2 2	
2.760E-04	2.710E-02	30	G313	2 1 1 2 2	

1259. C₇H₁₄

Methylcyclohexane

Hexahydrotoluene

Methyl cyclohexane

RN: 108-87-2**MP (°C):** -126**MW:** 98.19**BP (°C):** 101

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.222E-04	2.182E-02	2.34	S461	0 0 0 0 0	
2.000E-04	1.964E-02	9.99	S461	0 0 0 0 0	
1.711E-04	1.680E-02	20	B318	0 0 0 0 0	EFG
1.691E-04	1.660E-02	20	B356	0 0 0 0 0	
1.324E-04	1.300E-02	20	M337	2 1 2 2 2	
1.667E-04	1.636E-02	24.99	S461	0 0 0 0 0	
1.701E-04	1.670E-02	25	G313	2 1 1 2 2	
1.629E-04	1.600E-02	25	K119	1 0 0 0 2	

(continued)

1259. C₇H₁₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	1.400E-02	25	M001	2 1 2 2 2	
1.426E-04	1.400E-02	25	M002	2 1 2 2 2	
1.629E-04	1.600E-02	25.0	P051	2 1 1 2 2	
1.629E-04	1.600E-02	25.00	P007	2 1 2 2 2	
1.644E-04	1.615E-02	26.1	M447	0 0 0 0 0	
1.375E-04	1.350E-02	28	B348	2 1 2 2 2	
1.833E-04	1.800E-02	40.1	P051	2 1 1 2 2	
1.833E-04	1.800E-02	40.10	P007	2 1 2 2 2	
1.925E-04	1.890E-02	55.7	P051	2 1 1 2 2	
1.925E-04	1.890E-02	55.70	P007	2 1 2 2 2	
2.800E-04	2.749E-02	70.5	M447	0 0 0 0 0	
3.442E-04	3.380E-02	99.1	P051	2 1 1 2 2	
3.442E-04	3.380E-02	99.10	P007	2 1 2 2 2	
5.589E-04	5.487E-02	100.5	M447	0 0 0 0 0	
8.097E-04	7.950E-02	120.0	P051	2 1 1 2 2	
8.097E-04	7.950E-02	120.00	P007	2 1 2 2 2	
1.355E-03	1.331E-01	131.0	M447	0 0 0 0 0	
1.416E-03	1.390E-01	137.3	P051	2 1 1 2 2	
1.416E-03	1.390E-01	137.30	P007	2 1 2 2 2	
2.485E-03	2.440E-01	149.5	P051	2 1 1 2 2	
2.485E-03	2.440E-01	149.50	P007	2 1 2 2 2	
2.349E-03	2.307E-01	151.4	M447	0 0 0 0 0	
1.426E-04	1.400E-02	ns	H123	0 0 0 0 0	

1260. C₇H₁₄N₂O₂S

Aldicarb

Temik

2-Methyl-2-(methylthio)propanal O-[(methylamino)carbonyl]oxime

UC 21149

N-Methylcarbamoyloxime,2-methyl-2-methylsulfenylpropionaldehyde

Methylcarbamic acid

RN: 116-06-3 MP (°C): 99

MW: 190.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-02	6.017E+00	20	B179	0 0 0 0 0	
3.153E-02	6.000E+00	ns	H042	0 0 0 0 2	
3.135E-02	5.964E+00	ns	M061	0 0 0 0 0	
3.153E-02	6.000E+00	rt	M161	0 0 0 0 0	

1261. C₇H₁₄N₂O₃

ϵ -Aminocaproic hydantoic acid
 ϵ -Uramidocaproic acid

RN: MP (°C):
 MW: 174.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.202E+00	25	M024	1 2 0 1 2	

1262. C₇H₁₄N₂O₃

α -Aminocaproic hydantoic acid
 α -Uramidocaproic acid

RN: MP (°C): 169
 MW: 174.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-03	1.202E+00	25	M024	1 2 0 1 2	

1263. C₇H₁₄N₂O₄S₂

Djenkoic acid
 Djenkolsaeure

RN: 498-59-9 MP (°C):
 MW: 254.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.966E-02	5.000E+00	100	F300	1 0 0 0 0	

1264. C₇H₁₄N₆

N₂,N₂,N₄,N₄-Tetramethylmelamine
 Tetramethylmelamine

RN: 2827-47-6 MP (°C): 227.0
 MW: 182.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.052E-03	3.740E-01	25	C051	1 2 1 1 2	pH 7

1265. C₇H₁₄O

Cycloheptanol

RN: 502-41-0 MP (°C):
 MW: 114.19 BP (°C): 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-01	1.505E+01	ns	S460	0 0 0 0 0	

1266. C₇H₁₄O

Heptyl aldehyde

Heptanal

Oenanthaldehyd

RN: 111-71-7**MP (°C):** -43.3**MW:** 114.19**BP (°C):** 152.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.715E-02	3.100E+00	0	F300	1 0 0 0 1	
1.576E-02	1.800E+00	40	F300	1 0 0 0 1	

1267. C₇H₁₄O

4-Methyl-cyclohexanol

RN: 589-91-3**MP (°C):** -41**MW:** 114.19**BP (°C):** 171-173

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-01	1.505E+01	ns	S460	0 0 0 0 0	

1268. C₇H₁₄O

Dipropyl ketone

4-Heptanone

RN: 123-19-3**MP (°C):** -32.6**MW:** 114.19**BP (°C):** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.430E-02	7.342E+00	0	G032	1 2 1 1 2	
4.660E-02	5.321E+00	10	G032	1 2 1 1 2	
3.750E-02	4.282E+00	20	D052	1 1 0 0 1	
2.793E-02	3.190E+00	25.50	O005	2 0 2 2 1	
3.350E-02	3.825E+00	30	G032	1 2 1 1 2	
2.880E-02	3.289E+00	50	G032	1 2 1 1 2	
2.720E-02	3.106E+00	75	G032	1 2 1 1 2	

1269. C₇H₁₄O

2-Heptanone

Heptan-2-one

RN: 110-43-0**MP (°C):** -31**MW:** 114.19**BP (°C):** 151.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.489E-02	3.984E+00	20	D052	1 1 0 0 0	
3.836E-02	4.381E+00	20	G030	1 2 0 0 1	
3.800E-02	4.339E+00	20	M312	1 0 0 0 1	
3.750E-02	4.282E+00	25	G030	1 2 0 0 1	
1.675E-01	1.913E+01	25	P055	1 0 0 0 1	
3.570E-02	4.077E+00	25	W300	2 2 2 2 2	
3.489E-02	3.984E+00	30	G030	1 2 0 0 1	

1270. C₇H₁₄O

5-Methyl-2-hexanone

Methyl isoamyl ketone

Isopentyl methyl ketone

Methylhexanone

Methyl isoamyl ketone

MIAK

RN: 110-12-3 **MP (°C):** -74
MW: 114.19 **BP (°C):** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.677E-02	5.341E+00	ns	S460	0 0 0 0 0	

1271. C₇H₁₄O

2,4-Dimethyl-3-pentanone

2,4-Dimethylpentanone-3

RN: 565-80-0 **MP (°C):** -80
MW: 114.19 **BP (°C):** 124

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.137E-02	5.865E+00	20	G030	1 2 0 0 1	
4.963E-02	5.668E+00	25	G030	1 2 0 0 1	
4.877E-02	5.569E+00	30	G030	1 2 0 0 1	
4.972E-02	5.677E+00	ns	J300	0 0 0 0 0	

1272. C₇H₁₄O₂

Heptoic acid

Heptanoic acid

n-Heptanoic acid

RN: 111-14-8 **MP (°C):**
MW: 130.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.459E-02	1.900E+00	0	B136	1 0 2 1 2	
1.843E-02	2.400E+00	15	F300	1 0 0 0 1	
1.847E-02	2.404E+00	15	L006	1 0 0 0 2	
1.721E-02	2.240E+00	20	B136	1 0 2 1 2	
1.870E-02	2.434E+00	20.0	R001	1 1 1 1 2	
2.161E-02	2.813E+00	25	H122	1 0 0 0 2	
2.082E-02	2.710E+00	30	B136	1 0 2 1 2	
2.076E-02	2.703E+00	30.0	R001	1 1 1 1 2	
2.389E-02	3.110E+00	45	B136	1 0 2 1 2	
2.381E-02	3.100E+00	45.0	R001	1 1 1 1 2	
2.711E-02	3.530E+00	60	B136	1 0 2 1 2	
2.702E-02	3.518E+00	60.0	R001	1 1 1 1 2	
1.457E-02	1.896E+00	.0	R001	1 1 1 1 2	

1273. C₇H₁₄O₂

Pentyl acetate

Amyl acetate

RN: 628-63-7

MP (°C): -100

MW: 130.19

BP (°C): 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.304E-02	1.697E+00	20	D052	1 1 0 0 1	
1.290E-02	1.679E+00	20	S006	1 0 0 0 2	
1.329E-02	1.730E+00	25	K072	1 0 1 1 1	
1.329E-02	1.730E+00	25	M087	1 1 2 1 2	
3.060E-02	3.984E+00	30	R318	1 1 0 1 0	

1274. C₇H₁₄O₂Isopropyl *N*-butyrate

Isopropyl butyrate

N-Butyric acid isopropyl ester

RN: 638-11-9 MP (°C):

MW: 130.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.198E-02	1.560E+00	ns	J300	0 0 0 0 0	

1275. C₇H₁₄O₂

3-Hydroxy-5-methyl-5-ethyltetrahydrofuran

3-Furanol, 5-ethyltetrahydro-5-methyl-

RN: 30010-08-3 MP (°C):

MW: 130.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.983E-01	9.091E+01	rt	B066	0 2 0 0 1	

1276. C₇H₁₄O₂

Isoamyl acetate

Acetic acid isoamyl ester

Essigsaeureisoamyl ester

RN: 123-92-2 MP (°C): -79

MW: 130.19 BP (°C): 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	2.500E+00	15	F300	1 0 0 0 1	
1.222E-02	1.591E+00	20	E002	1 0 0 0 1	
1.227E-02	1.597E+00	23.50	O005	2 0 2 2 1	
1.533E-02	1.996E+00	25	L062	2 2 0 1 0	

1277. C₇H₁₄O₂

Methyl hexanoate

Methyl caproate

RN: 106-70-7

MP (°C): -71.0

MW: 130.19

BP (°C): 151.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E-02	1.325E+00	20	M337	2 1 2 2 2	

1278. C₇H₁₄O₂

Ethyl pentanoate

Ethyl *n*-valerate

Ethyl valerianate

RN: 539-82-2

MP (°C):

MW: 130.19

BP (°C): 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-02	2.226E+00	ns	S460	0 0 0 0 0	

1279. C₇H₁₄O₂*n*-Butyl propionate

Butyl propionate

RN: 590-01-2

MP (°C): -89

MW: 130.19

BP (°C): 146.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-02	1.498E+00	20	D052	1 1 0 0 0	
9.500E-03	1.237E+00	25	K012	1 0 0 0 1	
1.514E-02	1.970E+00	ns	S460	0 0 0 0 0	

1280. C₇H₁₄O₂

Propyl butyrate

Buttersaeure-propyl ester

n-Propyl *n*-butyrate

RN: 105-66-8

MP (°C): -95

MW: 130.19

BP (°C): 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-02	1.614E+00	17	F001	1 0 1 0 2	
1.244E-02	1.620E+00	17	F300	1 0 0 0 2	
1.200E-02	1.562E+00	17	S006	1 0 0 0 1	

1281. C₇H₁₄O₂*sec*-Amyl acetate

2-Pentyl acetate

1-Methylbutyl acetate

RN: 53496-15-4 MP (°C):

MW: 130.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.457E-02	1.896E+00	20	D052	1 1 0 0 0	

1282. C₇H₁₄O₃*n*-Ethyl β-ethoxypropionate

Ethyl β-ethoxypropionate

RN: 763-69-9 MP (°C):

MW: 146.19 BP (°C): 166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.597E-01	5.258E+01	25	D002	1 2 1 1 2	
3.566E-01	5.213E+01	25	R034	0 0 0 0 1	

1283. C₇H₁₄O₃

Butyl lactate

Butyl α-hydroxypropionate

2-Propanoic acid

Lactic acid butyl ester

Butyl 2-hydroxypropanoate

RN: 138-22-7 MP (°C): -28

MW: 146.19 BP (°C): 185

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.631E-01	3.846E+01	20	D052	1 1 0 0 1	
2.982E-01	4.360E+01	25	R006	2 2 0 1 2	

1284. C₇H₁₄O₃*n*-Propyl β-methoxypropionate

Propionic acid, 3-methoxy-, propyl ester

RN: 5349-56-4 MP (°C):

MW: 146.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.121E-01	3.101E+01	25	R034	0 0 0 0 1	

1285. C₇H₁₄O₃Methyl β -n-propoxypropionate

Propanoic acid, 3-propoxy-, methyl ester

RN: 14144-39-9 **MP (°C):****MW:** 146.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.249E-01	3.288E+01	25	R034	0 0 0 0 1	

1286. C₇H₁₄O₃

3-Methoxy butyl acetate

3-Methoxy-1-butanol acetate

Methyl-1,3-butylene glycol acetate

3-Methoxybutyl acetate

Butoxyl

Butoxyl (3-methoxy-N-butyl acetate)

RN: 4435-53-4 **MP (°C):****MW:** 146.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.151E-01	6.068E+01	20	D052	1 1 0 0 2	

1287. C₇H₁₄O₆ β -Methyl-D-glucoside β -Methyl-D-glucosid**RN:** 709-50-2 **MP (°C):****MW:** 194.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.892E+00	3.674E+02	17	F300	1 0 0 0 2	

1288. C₇H₁₄O₆ α -D-Methylglucoside α -Methyl-D-glucoside α -Methyl-D-glucosid**RN:** 97-30-3 **MP (°C):** 168**MW:** 194.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E+00	3.868E+02	17	F300	1 0 0 0 2	
2.543E+00	4.938E+02	17.8	W013	1 2 1 1 2	
2.637E+00	5.120E+02	22.5	W013	1 2 1 1 2	
2.657E+00	5.159E+02	25.5	W013	1 2 1 1 2	
2.696E+00	5.236E+02	26.6	W013	1 2 1 1 2	
2.699E+00	5.241E+02	27.3	W013	1 2 1 1 2	

(continued)

1288. C₇H₁₄O₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.751E+00	5.342E+02	31.8	W013	1 2 1 1 2	
2.806E+00	5.448E+02	33.9	W013	1 2 1 1 2	
2.849E+00	5.533E+02	37.2	W013	1 2 1 1 2	
2.951E+00	5.731E+02	43.2	W013	1 2 1 1 2	
3.060E+00	5.942E+02	49.0	W013	1 2 1 1 2	
3.078E+00	5.978E+02	49.6	W013	1 2 1 1 2	
3.131E+00	6.079E+02	51.8	W013	1 2 1 1 2	
3.166E+00	6.148E+02	54.4	W013	1 2 1 1 2	
3.213E+00	6.240E+02	57.3	W013	1 2 1 1 2	
3.297E+00	6.402E+02	60.6	W013	1 2 1 1 2	
3.332E+00	6.471E+02	62.7	W013	1 2 1 1 2	
3.360E+00	6.525E+02	64.2	W013	1 2 1 1 2	
3.403E+00	6.608E+02	66.2	W013	1 2 1 1 2	
3.435E+00	6.670E+02	67.8	W013	1 2 1 1 2	
3.542E+00	6.878E+02	73.2	W013	1 2 1 1 2	
3.651E+00	7.090E+02	78.0	W013	1 2 1 1 2	

1289. C₇H₁₄O₆ α -Methyl-D-mannoside α -Methyl-D-mannosid

RN: 617-04-9

MP (°C):

MW: 194.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.018E+00	1.976E+02	17	F300	1 0 0 0 2	

1290. C₇H₁₄O₇

D-Mannoheptose

D-Sedoheptose

RN: 7634-39-1

MP (°C):

MW: 210.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>4.76E-01	>1.00E+02	20	F300	1 0 0 0 0	

1291. C₇H₁₄O₇D- α -Glucoheptose

Gluco-heptose

RN: 62475-58-5

MP (°C):

MW: 210.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-01	8.676E+01	20	D041	1 0 0 0 1	

1292. C₇H₁₅Br

1-Bromoheptane

Heptyl bromide

RN: 629-04-9

MP (°C): -56.1

MW: 179.11

BP (°C): 178.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.710E-05	6.645E-03	25	M342	1 0 1 1 2	

1293. C₇H₁₅Cl

1-Chloroheptane

Heptyl chloride

RN: 629-06-1

MP (°C): -69.5

MW: 134.65

BP (°C): 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-04	1.360E-02	25	M342	1 0 1 1 2	

1294. C₇H₁₅Cl₂N₂O₂P

Cyclophosphamide

Cyclophosphoramide

2-(bis(2-Chloroethyl)-amino)tetrahydro-2H-1,3,2-oxazaphosphorine 2-oxide

Cycloblastin

Sendoxan

Claphene

RN: 50-18-0

MP (°C):

MW: 261.09

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.532E-01	4.000E+01	ns	K444	0 0 0 0 0	

1295. C₇H₁₅I

1-Iodoheptane

Heptyl iodide

RN: 4282-40-0

MP (°C): -48.2

MW: 226.10

BP (°C): 204

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-05	3.505E-03	25	M342	1 0 1 1 2	

1296. C₇H₁₅NO₂

Isobutyl urethane

Isobutylurethan

RN: 539-89-9 **MP (°C):**
MW: 145.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-01	2.482E+01	15.5	F001	1 0 1 2 2	

1297. C₇H₁₅NO₂

n-Hexyl carbamate

Hexyl carbamate

RN: 2114-20-7 **MP (°C):** 62
MW: 145.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	1.742E+00	37	H006	1 2 2 1 1	

1298. C₇H₁₅NO₂

tert-Hexyl carbamate

3,3-Dimethyl-1-butanol carbamate

RN: 3124-38-7 **MP (°C):**
MW: 145.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-02	4.937E+00	37	H006	1 2 2 1 1	

1299. C₇H₁₆

3,3-Dimethylpentane

3,3-Dwumetylpentan

RN: 562-49-2 **MP (°C):** -135
MW: 100.21 **BP (°C):** 86

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.928E-05	5.940E-03	25	K119	1 0 0 0 2	
5.908E-05	5.920E-03	25.0	P051	2 1 1 2 2	
5.908E-05	5.920E-03	25.00	P007	2 1 2 2 2	
6.766E-05	6.780E-03	40.1	P051	2 1 1 2 2	
6.766E-05	6.780E-03	40.10	P007	2 1 2 2 2	
8.153E-05	8.170E-03	55.7	P051	2 1 1 2 2	
8.153E-05	8.170E-03	55.70	P007	2 1 2 2 2	
1.028E-04	1.030E-02	69.7	P051	2 1 1 2 2	
1.028E-04	1.030E-02	69.70	P007	2 1 2 2 2	
1.577E-04	1.580E-02	99.1	P051	2 1 1 2 2	

(continued)

1299. C₇H₁₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.577E-04	1.580E-02	99.10	P007	2 1 2 2 2	
2.724E-04	2.730E-02	118.0	P051	2 1 1 2 2	
2.724E-04	2.730E-02	118.00	P007	2 1 2 2 2	
6.716E-04	6.730E-02	120.4	P051	2 1 1 2 2	
6.716E-04	6.730E-02	120.40	P007	2 1 2 2 2	
8.592E-04	8.610E-02	150.4	P051	2 1 1 2 2	
8.592E-04	8.610E-02	150.40	P007	2 1 2 2 2	

1300. C₇H₁₆

3-Methylhexane

3-Metyloheksan

RN: 589-34-4

MP (°C): -119

MW: 100.21

BP (°C): 91

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.229E-05	5.240E-03	0	P003	2 2 2 2 2	
1.048E-04	1.050E-02	23	C332	0 0 0 0 0	
2.635E-05	2.640E-03	25	K119	1 0 0 0 2	
4.940E-05	4.950E-03	25	P003	2 2 2 2 2	
2.635E-05	2.640E-03	25	P051	2 1 1 2 2	
2.635E-05	2.640E-03	25.00	P007	2 1 2 2 2	

1301. C₇H₁₆

2,4-Dimethylpentane

2,4-Dwumetylopentan

RN: 108-08-7

MP (°C): -123

MW: 100.21

BP (°C): 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.487E-05	6.500E-03	0	P003	2 2 2 2 2	
4.401E-05	4.410E-03	25	K119	1 0 0 0 2	
4.052E-05	4.060E-03	25	M001	2 1 2 2 2	
3.613E-05	3.620E-03	25	M002	2 1 2 2 2	
5.489E-05	5.500E-03	25	P003	2 2 2 2 2	
4.401E-05	4.410E-03	25	P051	2 1 1 2 2	
4.401E-05	4.410E-03	25.00	P007	2 1 2 2 2	
4.100E-05	4.108E-03	ns	J300	0 0 0 0 0	

1302. C₇H₁₆

2,3-Dimethylpentane

2,3-Dwumetylopentan

RN: 565-59-3 **MP (°C):** <25
MW: 100.21 **BP (°C):** 89

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.239E-05	5.250E-03	25	K119	1 0 0 0 2	
5.239E-05	5.250E-03	25	P051	2 1 1 2 2	
5.239E-05	5.250E-03	25.00	P007	2 1 2 2 2	

1303. C₇H₁₆

2-Methylhexane

2-Metyloheksan

RN: 591-76-4 **MP (°C):** -118
MW: 100.21 **BP (°C):** 90

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-04	1.400E-02	23	C332	0 0 0 0 0	
2.535E-05	2.540E-03	25	K119	1 0 0 0 2	
2.535E-05	2.540E-03	25	P051	2 1 1 2 2	
2.535E-05	2.540E-03	25.00	P007	2 1 2 2 2	

1304. C₇H₁₆

2,2-Dimethylpentane

2,2-Dwumetylopentan

RN: 590-35-2 **MP (°C):** -123
MW: 100.21 **BP (°C):** 79.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.391E-05	4.400E-03	25	K119	1 0 0 0 2	
4.391E-05	4.400E-03	25	P051	2 1 1 2 2	
4.391E-05	4.400E-03	25.00	P007	2 1 2 2 2	
4.100E-05	4.108E-03	ns	J300	0 0 0 0 0	

1305. C₇H₁₆

Heptane

n-Heptane

RN: 142-82-5 **MP (°C):** -90.7
MW: 100.21 **BP (°C):** 98.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.381E-05	4.390E-03	0	P003	2 2 2 2 2	
8.333E-05	8.350E-03	2.34	S461	0 0 0 0 0	

(continued)

1305. C₇H₁₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-05	1.954E-03	4.3	N004	1 1 2 2 2	
1.667E-05	1.670E-03	9.99	S461	0 0 0 0 0	
2.017E-05	2.021E-03	13.5	N004	1 1 2 2 2	
4.990E-04	5.000E-02	15	F300	1 0 0 0 1	
5.200E-04	5.211E-02	15.50	F001	1 0 1 0 2	
1.497E-04	1.500E-02	16	D047	1 0 0 1 0	
2.694E-05	2.700E-03	20	M337	2 1 2 2 1	
1.111E-05	1.113E-03	24.99	S461	0 0 0 0 0	
3.990E-03	3.998E-01	25	G323	2 2 2 2 0	
4.990E-04	5.000E-02	25	K072	1 0 1 1 1	
2.235E-05	2.240E-03	25	K119	1 0 0 0 2	
2.924E-05	2.930E-03	25	M001	2 1 2 2 2	
2.924E-05	2.930E-03	25	M002	2 1 2 2 2	
4.990E-04	5.000E-02	25	M087	1 1 2 1 0	
3.050E-05	3.056E-03	25	M342	1 0 1 1 2	
3.363E-05	3.370E-03	25	P003	2 2 2 2 2	
4.989E-04	5.000E-02	25	S012	2 0 2 2 0	
2.656E-05	2.661E-03	25.0	N004	1 1 2 2 2	
2.235E-05	2.240E-03	25.0	P051	2 1 1 2 2	
2.235E-05	2.240E-03	25.00	P007	2 1 2 2 2	
2.261E-05	2.266E-03	35.0	N004	1 1 2 2 2	
2.625E-05	2.630E-03	40.1	P051	2 1 1 2 2	
2.400E-05	2.405E-03	45.0	N004	1 1 2 2 2	
8.973E-03	8.992E-01	50	G323	2 2 2 2 0	
3.104E-05	3.110E-03	55.7	P051	2 1 1 2 2	
3.104E-05	3.110E-03	55.70	P007	2 1 2 2 2	
5.589E-05	5.600E-03	99.1	P051	2 1 1 2 2	
5.589E-05	5.600E-03	99.10	P007	2 1 2 2 2	
1.138E-04	1.140E-02	118	P007	2 1 2 2 2	
1.138E-04	1.140E-02	118.0	P051	2 1 1 2 2	
2.724E-04	2.730E-02	136.6	P051	2 1 1 2 2	
2.724E-04	2.730E-02	136.60	P007	2 1 2 2 2	
4.361E-04	4.370E-02	150.4	P051	2 1 1 2 2	
4.361E-04	4.370E-02	150.40	P007	2 1 2 2 2	
3.692E-05	3.700E-03	ns	B151	0 2 1 1 1	
7.000E-04	7.014E-02	ns	H012	0 2 2 0 0	

1306. C₇H₁₆O

3-Heptanol

(±)-3-Heptanol

3-Hydroxyheptane

1-Ethyl-1-pentanol

RN: 589-82-2

MP (°C): -70

MW: 116.20

BP (°C): 156.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-02	4.764E+00	20	H330	0 0 0 0 0	
3.428E-02	3.984E+00	25	C093	2 1 1 1 0	

1307. C₇H₁₆O

2-Heptanol

2-Hydroxyheptane

Amylmethylcarbinol

RN: 543-49-7

MP (°C): <25

MW: 116.20

BP (°C): 159.00

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.532E-02	6.428E+00	0	S307	1 1 0 2 2	
3.966E-02	4.609E+00	10.2	S307	1 1 0 2 2	
3.633E-02	4.222E+00	19.5	S307	1 1 0 2 2	
3.001E-02	3.488E+00	30.7	S307	1 1 0 2 2	
2.813E-02	3.269E+00	40.0	S307	1 1 0 2 2	
2.514E-02	2.921E+00	50.0	S307	1 1 0 2 2	
2.471E-02	2.872E+00	60.3	S307	1 1 0 2 2	
2.754E-02	3.200E+00	70.3	S307	1 1 0 2 2	
2.754E-02	3.200E+00	80.0	S307	1 1 0 2 2	
2.942E-02	3.418E+00	90.2	S307	1 1 0 2 2	

1308. C₇H₁₆O

3-Methyl-3-hexanol

3-Methylhexanol-3

RN: 597-96-6

MP (°C): <25

MW: 116.20

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.146E-01	1.332E+01	20	G006	1 2 1 1 2	
1.012E-01	1.176E+01	25	G006	1 2 1 1 2	
9.110E-02	1.059E+01	30	G006	1 2 1 1 2	

1309. C₇H₁₆O

3-Ethyl-3-pentanol

3-Ethyl-pentanol-3

Triethyl carbinol

RN: 597-49-9

MP (°C): -12

MW: 116.20

BP (°C): 141.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.613E-01	1.874E+01	20	G006	1 2 1 1 2	
1.422E-01	1.652E+01	25	G006	1 2 1 1 2	
1.272E-01	1.478E+01	30	G006	1 2 1 1 2	
1.071E-01	1.244E+01	40	G006	1 2 1 1 2	

1310. C₇H₁₆O

2-Methyl-2-hexanol

2-Methylhexanol-2

RN: 625-23-0 **MP (°C):** <25
MW: 116.20 **BP (°C):** 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.195E-02	1.068E+01	20	G006	1 2 1 1 2	
8.267E-02	9.607E+00	25	G006	1 2 1 1 1	
7.422E-02	8.625E+00	30	G006	1 2 1 1 1	

1311. C₇H₁₆O

2,4-Dimethyl-3-pentanol

2,4-Dimethylpentanol-3

Diisopropyl carbinol

RN: 600-36-2 **MP (°C):** -70
MW: 116.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	1.172E+01	0	S307	1 1 0 2 2	
8.942E-02	1.039E+01	10.0	S307	1 1 0 2 2	
6.660E-02	7.740E+00	20	G006	1 2 1 1 1	
6.067E-02	7.050E+00	20.2	S307	1 1 0 2 2	
1.935E-01	2.248E+01	24.50	O005	2 0 2 2 1	
5.982E-02	6.951E+00	25	G006	1 2 1 1 1	
5.727E-02	6.655E+00	30	G006	1 2 1 1 1	
5.489E-02	6.379E+00	30.6	S307	1 1 0 2 2	
4.562E-02	5.302E+00	39.5	S307	1 1 0 2 2	
4.332E-02	5.035E+00	49.7	S307	1 1 0 2 2	
3.992E-02	4.638E+00	60.3	S307	1 1 0 2 2	
3.778E-02	4.391E+00	70.2	S307	1 1 0 2 2	
3.667E-02	4.262E+00	80.2	S307	1 1 0 2 2	
3.855E-02	4.480E+00	90.6	S307	1 1 0 2 2	

1312. C₇H₁₆O

2,4-Dimethyl-2-pentanol

2,4-Dimethylpentanol-2

RN: 625-06-9 **MP (°C):** <-20
MW: 116.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.272E-01	1.478E+01	20	G006	1 2 1 1 2	
1.138E-01	1.322E+01	25	G006	1 2 1 1 2	
1.037E-01	1.205E+01	30	G006	1 2 1 1 2	

1313. C₇H₁₆O

2,3-Dimethyl-2-pentanol

2,3-Dimethylpentanol-2

RN: 4911-70-0 MP (°C): <25

MW: 116.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-01	1.662E+01	20	G006	1 2 1 1 2	
1.305E-01	1.517E+01	25	G006	1 2 1 1 2	
1.188E-01	1.381E+01	30	G006	1 2 1 1 2	

1314. C₇H₁₆O

2,3,3-Trimethyl-2-butanol

Dimethyl-*tert*-butylcarbinol

1,1,2,2-Tetramethylpropanol

1,1,2,2-Tetramethylpropyl alcohol

RN: 594-83-2 MP (°C): 17

MW: 116.20 BP (°C): 131

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.852E-01	2.153E+01	40	G006	1 2 1 1 2	

1315. C₇H₁₆O

2,2-Dimethyl-3-pentanol

2,2-Dimethylpentanol-3

RN: 3970-62-5 MP (°C): -5

MW: 116.20 BP (°C): 132

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.507E-02	8.723E+00	20	G006	1 2 1 1 1	
6.999E-02	8.133E+00	25	G006	1 2 1 1 1	
6.745E-02	7.838E+00	30	G006	1 2 1 1 1	

1316. C₇H₁₆O

1-Heptanol

1-Hydroxyheptane

Heptan-1-ol

Heptanol-(1)

n-Heptyl alcohol

RN: 111-70-6 MP (°C): -34.6

MW: 116.20 BP (°C): 175.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.916E-02	3.388E+00	0	E029	1 2 0 1 1	
2.026E-02	2.354E+00	0	S307	1 1 0 2 2	
1.897E-02	2.205E+00	6.04	H110	2 2 2 2 2	

(continued)

1316. C₇H₁₆O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.232E-02	2.593E+00	10	E029	1 2 0 1 1	
1.739E-02	2.020E+00	10.24	H110	2 2 2 2 2	
2.172E-02	2.524E+00	10.5	S307	1 1 0 2 2	
1.720E-02	1.999E+00	10.54	H110	2 2 2 2 2	
1.067E-02	1.240E+00	11.4	N042	1 0 2 1 1	
1.608E-02	1.869E+00	15.04	H110	2 2 2 2 2	
1.544E-02	1.795E+00	17.94	H110	2 2 2 2 2	
8.000E-03	9.296E-01	18	F001	1 0 1 0 2	
8.605E-03	1.000E+00	18	F300	1 0 0 0 1	
1.478E-02	1.717E+00	20	A015	1 2 1 1 2	
1.718E-02	1.996E+00	20	E029	1 2 0 1 1	
1.450E-02	1.685E+00	20	H330	0 0 0 0 0	
1.507E-02	1.751E+00	20.04	H110	2 2 2 2 2	
1.581E-02	1.837E+00	20.2	S307	1 1 0 2 2	
1.476E-02	1.716E+00	21.94	H110	2 2 2 2 2	
1.450E-02	1.685E+00	23.94	H110	2 2 2 2 2	
1.443E-02	1.677E+00	24.94	H110	2 2 2 2 2	
1.546E-02	1.797E+00	25	B038	1 2 1 1 2	
1.000E+00	1.162E+02	25	F044	1 0 0 0 0	EFG
1.460E-02	1.697E+00	25	K025	2 1 1 1 1	
1.434E-02	1.666E+00	25.04	H110	2 2 2 2 2	
1.423E-02	1.653E+00	26.04	H110	2 2 2 2 2	
1.411E-02	1.640E+00	28.04	H110	2 2 2 2 2	
1.375E-02	1.597E+00	30	E029	1 2 0 1 1	
1.397E-02	1.624E+00	30.14	H110	2 2 2 2 2	
1.399E-02	1.626E+00	30.14	H110	2 2 2 2 2	
1.323E-02	1.538E+00	30.6	S307	1 1 0 2 2	
1.386E-02	1.611E+00	32.94	H110	2 2 2 2 2	
1.426E-02	1.657E+00	39.8	S307	1 1 0 2 2	
1.117E-02	1.298E+00	40	E029	1 2 0 1 1	
9.456E-03	1.099E+00	50	E029	1 2 0 1 1	
1.392E-02	1.617E+00	50.1	S307	1 1 0 2 2	
9.456E-03	1.099E+00	60	E029	1 2 0 1 1	
1.529E-02	1.777E+00	60.0	S307	1 1 0 2 2	
1.289E-02	1.498E+00	70	E029	1 2 0 1 1	
1.080E-02	1.255E+00	70	F001	1 0 1 0 2	
1.752E-02	2.036E+00	70.1	S307	1 1 0 2 2	
1.632E-02	1.896E+00	80	E029	1 2 0 1 1	
1.460E-02	1.697E+00	80	F001	1 0 1 0 2	
1.863E-02	2.165E+00	80.1	S307	1 1 0 2 2	
1.975E-02	2.295E+00	90	E029	1 2 0 1 1	
1.940E-02	2.254E+00	90	F001	1 0 1 0 2	
2.086E-02	2.424E+00	90.5	S307	1 1 0 2 2	
2.488E-02	2.892E+00	100	E029	1 2 0 1 1	
2.460E-02	2.859E+00	100	F001	1 0 1 0 2	
2.582E-02	3.000E+00	100	F300	1 0 0 0 1	
3.001E-02	3.488E+00	110	E029	1 2 0 1 1	
3.060E-02	3.556E+00	110	F001	1 0 1 0 2	
3.685E-02	4.282E+00	120	E029	1 2 0 1 1	

(continued)

1316. C₇H₁₆O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.537E-02	5.272E+00	130	E029	1 2 0 1 1	
5.557E-02	6.458E+00	140	E029	1 2 0 1 1	
6.830E-02	7.937E+00	150	E029	1 2 0 1 1	
8.352E-02	9.705E+00	160	E029	1 2 0 1 1	
1.046E-01	1.215E+01	170	E029	1 2 0 1 2	
1.355E-01	1.575E+01	180	E029	1 2 0 1 2	
1.753E-01	2.038E+01	190	E029	1 2 0 1 2	
2.213E-01	2.572E+01	200	E029	1 2 0 1 2	
2.894E-01	3.363E+01	210	E029	1 2 0 1 2	
3.847E-01	4.471E+01	220	E029	1 1 0 1 2	
5.404E-01	6.279E+01	230	E029	1 2 0 1 2	
7.894E-01	9.173E+01	240	E029	1 2 0 1 2	
1.054E+00	1.225E+02	245	E029	1 2 0 1 2	
1.029E-02	1.195E+00	ns	H012	0 2 2 0 2	
1.558E-02	1.810E+00	ns	L003	0 0 2 1 2	

1317. C₇H₁₆OIsopropyl *tert*-butyl ether

2-Methyl-2-(1-methylethoxy)-propane

t-Butyl isopropyl ether

RN: 17348-59-3 MP (°C): -88
 MW: 116.20 BP (°C): 87.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.303E-03	5.000E-01	25	K072	1 0 1 1 1	
4.303E-03	5.000E-01	25	M087	1 1 2 1 1	

1318. C₇H₁₆O

Heptanol

RN: 53535-33-4 MP (°C): -36
 MW: 116.20 BP (°C): 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-01	1.173E+01	20	S006	1 0 0 0 2	
1.240E-02	1.441E+00	24	H345	0 0 0 0 0	

1319. C₇H₁₆O

4-Heptanol

Dipropyl carbinol

RN: 589-55-9 MP (°C): -42
 MW: 116.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.090E-02	4.753E+00	20	H330	0 0 0 0 0	

1320. C₇H₁₆O

2,3-Dimethyl-3-pentanol

2,3-Dimethylpentanol-3

RN: 595-41-5 **MP (°C):** <25
MW: 116.20 **BP (°C):** 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-01	1.836E+01	20	G006	1 2 1 1 2	
1.389E-01	1.614E+01	25	G006	1 2 1 1 2	
1.213E-01	1.410E+01	30	G006	1 2 1 1 2	

1321. C₇H₁₆O₄S₂

Sulfonmethane

Sulfonal

RN: 115-24-2 **MP (°C):** 125
MW: 228.33 **BP (°C):** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.962E-02	1.361E+01	16	A072	1 0 1 0 2	
5.956E-02	1.360E+01	16	F300	1 0 0 0 2	
1.027E-02	2.345E+00	18	F062	1 0 2 2 2	
2.847E-01	6.500E+01	100	F300	1 0 0 0 1	
5.888E-02	1.345E+01	ns	R427	0 0 0 0 0	

1322. C₇H₁₆O₇

(+) -Perseitol

D-Manno- α -heptit

RN: 527-06-0 **MP (°C):** 188
MW: 212.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.044E-01	6.460E+01	18	F300	1 0 0 0 2	
1.466E+00	3.110E+02	74	F300	1 0 0 0 1	

1323. C₇H₁₇O₂PS₃

Phorate

Thimet

Rampart

Phosphorodithioic acid *O,O*-diethyl *S*-[(ethylthio)methyl] ester

American Cyanamid 3911

CL 35024

RN: 298-02-2 **MP (°C):** -43
MW: 260.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.874E-05	1.790E-02	20	B169	2 1 1 1 1	
1.905E-04	4.961E-02	20	B179	0 0 0 0 0	

(continued)

1323. C₇H₁₇O₂PS₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.681E-05	2.000E-02	24	F179	2 2 2 2 2	
2.688E-04	7.000E-02	ns	M061	0 0 0 0 1	
1.920E-04	5.000E-02	rt	M161	0 0 0 0 1	

1324. C₇H₁₇O₂PS₃S-2-Isopropylthioethyl *O,O*-dimethyl phosphorodithioate

Isothioate

O,O-Dimethyls-isopropylthioethyl phosphoroditjioate

RN: 36614-38-7 MP (°C):

MW: 260.38 BP (°C): 55

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.725E-04	9.700E-02	25	M161	1 0 0 0 1	
3.725E-04	9.700E-02	25	N304	1 0 0 0 1	

1325. C₇H₁₇O₄PS₃

Phorate sulfone

O,O'-Diethyl S-ethylsulfonylmethyl-phosphorodithioate

Thimet sulfone

CL 18161

Phosphorodithioic acid *O,O*-diethyl S-[(ethylsulfonyl)methyl] ester

RN: 2588-04-7 MP (°C):

MW: 292.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.939E-03	8.593E-01	19	B169	2 0 1 1 2	

1326. C₈H₂Cl₄N₂

Chlorquinox

5,6,7,8-Tetrachloroquinoxaline

Lucel

Tetrachloroquinoxaline

RN: 3495-42-9 MP (°C): 190

MW: 267.93 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.732E-06	1.000E-03	25	M161	1 0 0 0 0	

1327. C₈H₂Cl₄O₄

Tetrachlorophthalic acid

Tetrachlorphthalsaeure

Tetrachloro-1,2-benzenedicarboxylic acid

RN: 632-58-6 **MP (°C):****MW:** 303.91 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.876E-02	5.700E+00	14	F300	1 0 0 0 1	
1.007E-01	3.060E+01	99	F300	1 0 0 0 2	

1328. C₈H₃Cl₂F₃N₂

Chlorflurazole

4,5-Dichloro-2-(trifluoromethyl)-benzimidazole

Dichloro-2-(trifluoromethyl)benzimidazole

2-Trifluoromethyl-4,5-dichlorobenzimidazole

RN: 3615-21-2 **MP (°C):****MW:** 255.03 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.353E-04	6.000E-02	ns	B100	0 0 0 0 0	
2.353E-04	6.000E-02	ns	M061	0 0 0 0 1	

1329. C₈H₃Cl₅O₂

Pentachlorophenyl acetate

Pentachlorophenol acetate

Rabcon

RN: 1441-02-7 **MP (°C):****MW:** 308.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.486E-05	2.000E-02	ns	L311	0 0 0 0 1	

1330. C₈H₃Cl₅O₃

2,3,4,5,6-Pentachlorophenoxyacetic acid

Pentachlorophenoxyacetic acid

RN: 2877-14-7 **MP (°C):****MW:** 324.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-04	5.839E-02	25	L030	1 0 2 1 1	

1331. C₈H₄Cl₄O₃

2,3,4,6-Tetrachlorophenoxyacetic acid

Acetic acid, (2,3,4,6-tetrachlorophenoxy)-

RN: 10587-37-8 MP (°C):

MW: 289.93 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	1.131E-01	25	L030	1 0 2 1 1	

1332. C₈H₄N₂

1,4-Benzenedicarbonitrile

Terephthalonitrile

1,4-Dicyanobenzene

RN: 623-26-7 MP (°C):

MW: 128.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.970E-04	8.931E-02	25	C316	0 0 0 0 0	0.1M NaCl

1333. C₈H₄N₂S*m*-Cyanophenyl isothiocyanate

3-Isothiocyanato-benzonitrile

3-Cyanophenyl isothiocyanate

RN: 3125-78-8 MP (°C):

MW: 160.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.410E-04	1.027E-01	25	K032	2 2 0 1 2	

1334. C₈H₄N₂S₂*m*-Isothiocyanophenyl isothiocyanate

3-Isothiocyanophenyl isothiocyanate

RN: 3125-77-7 MP (°C):

MW: 192.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	3.845E-03	25	K032	2 2 0 1 1	

1335. C₈H₄O₃

Phthalic anhydride

1,2-Benzenedicarboxylic acid anhydride

1,3-Isobenzofurandione

Phthalic acid anhydride

1,3-Dioxophthalan

1,3 Phthalandione

RN: 85-44-9

MP (°C): 130.8

MW: 148.12

BP (°C): 295.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.186E-02	6.200E+00	26.70	L095	2 2 1 1 2	
4.027E-02	5.964E+00	rt	D021	0 0 1 1 2	

1336. C₈H₅ClO₄

3-Chlorophthalic acid

3-Chlor-phthalsaeure

RN: 27563-65-1

MP (°C):

MW: 200.58

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E-01	2.120E+01	14	F300	1 0 0 0 2	

1337. C₈H₅Cl₃O₂

Chlorfenac

2,3,6-Trichlorophenylacetic acid

Fenac

RN: 85-34-7

MP (°C): 161

MW: 239.49

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.351E-04	2.000E-01	28	M161	1 0 0 0 2	
8.351E-04	2.000E-01	30	M061	1 0 0 0 2	

1338. C₈H₅Cl₃O₃

2,4,5-Trichlorophenoxyacetic acid

Acetic acid, (2,4,5-trichlorophenoxy)-

(2,4,5-Trichlorophenoxy)acetic acid

2,4,5-T

RN: 93-76-5

MP (°C): 156

MW: 255.49

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.316E-04	2.380E-01	20	B185	0 0 0 0 0	
7.398E-04	1.890E-01	20	M061	1 0 0 0 2	
1.090E-03	2.785E-01	24.99	N417	0 0 0 0 0	

(continued)

1338. C₈H₅Cl₃O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	2.810E-01	25	B164	1 0 1 1 2	
1.096E-03	2.800E-01	25	B185	0 0 0 0 0	
1.050E-03	2.683E-01	25	L030	1 0 2 1 2	
1.088E-03	2.780E-01	25	M161	1 0 0 0 2	
9.316E-04	2.380E-01	30	B200	1 0 0 0 2	
9.783E-04	2.499E-01	ns	B100	0 0 0 0 1	
7.828E-04	2.000E-01	ns	B185	0 0 0 0 0	
8.000E-04	2.044E-01	ns	F184	0 0 0 0 1	
9.316E-04	2.380E-01	ns	K138	0 0 0 0 1	
9.824E-04	2.510E-01	ns	L024	0 0 0 0 2	
2.512E-04	6.418E-02	ns	M163	0 0 0 0 0	EFG
7.828E-04	2.000E-01	ns	N013	0 0 0 0 2	

1339. C₈H₅Cl₃O₃

3,4,5-Trichlorophenoxyacetic acid
Acetic acid, (3,4,5-trichlorophenoxy)-
3,4,5-T

RN: 80496-87-3 **MP (°C):**
MW: 255.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-03	2.938E-01	25	L030	1 0 2 1 2	

1340. C₈H₅Cl₃O₃

2,3,4-Trichlorophenoxyacetic acid
Acetic acid, (2,3,4-trichlorophenoxy)-
2,3,4-T

RN: 25141-27-9 **MP (°C):**
MW: 255.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-04	2.044E-01	25	L030	1 0 2 1 1	

1341. C₈H₅Cl₃O₃

2,4,6-Trichlorophenoxyacetic acid
Acetic acid, (2,4,6-trichlorophenoxy)-
2,4,6-T

RN: 575-89-3 **MP (°C):** 45
MW: 255.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-04	2.478E-01	25	L030	1 0 2 1 1	

1342. C₈H₅Cl₃O₃

2,3,6-Trichlorophenoxyacetic acid
 Acetic acid, (2,3,6-trichlorophenoxy)-
 2,3,6-T

RN: 4007-00-5 **MP (°C):** 148
MW: 255.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-03	6.132E-01	25	L030	1 0 2 1 2	

1343. C₈H₅Cl₃O₃

2,3,5-Trichlorophenoxyacetic acid
 Acetic acid, (2,3,5-trichlorophenoxy)-
 2,3,5-T

RN: 33433-95-3 **MP (°C):**
MW: 255.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.555E-01	25	L030	1 0 2 1 2	

1344. C₈H₅F₃O

2,2,2-Trifluoroacetophenone

Trifluoroacetophenone

α,α,α-Trifluoroacetophenone

Phenyl trifluoromethyl ketone

2,2,2-Trifluoro-1-phenylethanone

RN: 434-45-7 **MP (°C):** -40

MW: 174.12 **BP (°C):** 165–166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.007E-02	1.220E+01	30	B433	0 0 0 0 0	

1345. C₈H₅F₃O₂

α,α,α-Trifluoro-*o*-toluic acid

Trifluoro-*o*-toluic acid

Acide orthotrifluortolueque

RN: 433-97-6 **MP (°C):** 111

MW: 190.12 **BP (°C):** 247

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.525E-02	4.800E+00	25	D064	1 2 1 1 2	

1346. C₈H₅NO₂

Phthalimide

Phthalimid

RN: 85-41-6

MP (°C): 238.0

MW: 147.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.447E-03	3.600E-01	25	F300	1 0 0 0 1	
2.719E-02	4.000E+00	100	F300	1 0 0 0 0	
4.075E-03	5.996E-01	rt	D021	0 0 1 1 0	

1347. C₈H₅NO₂S

3-Carboxyphenylisothiocyanate

m-Isothiocyanobenzoic acid

RN: 2131-63-7 MP (°C):

MW: 179.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-04	1.004E-01	25	D019	1 1 1 1 2	
8.000E-04	1.434E-01	25	K032	2 2 0 1 1	

1348. C₈H₅NO₂S

4-Carboxyphenylisothiocyanate

p-Carboxyphenylisothiocyanate

RN: 2131-62-6 MP (°C):

MW: 179.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-04	1.900E-02	25	D019	1 1 1 1 2	

1349. C₈H₅NO₄

6-Nitrophthalide

6-Nitro-phthalid

RN: 610-93-5 MP (°C): 145

MW: 179.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.233E-03	4.000E-01	25	F300	1 0 0 0 2	

1350. C₈H₅NO₆

3-Nitrophthalic acid

3-Nitro-phthalsaeure

RN: 603-11-2

MP (°C): 218

MW: 211.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.520E-02	2.010E+01	25	F300	1 0 0 0 2	

1351. C₈H₅NO₆

2,3,4-Pyridinetricarboxylic acid

Pyridin-tricarbonsaeure-(2,3,4)

RN: 632-95-1

MP (°C): 250

MW: 211.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.684E-02	1.200E+01	15	F300	1 0 0 0 1	

1352. C₈H₆

Ethynylbenzene

Phenylacetylene

RN: 536-74-3

MP (°C): -44.8

MW: 102.14

BP (°C): 142.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.467E-03	4.562E-01	ns	D001	0 0 0 0 2	

1353. C₈H₆BrNS

3-Bromobenzyl isothiocyanate

m-Bromobenzyl isothiocyanate

RN: 3845-33-8

MP (°C):

MW: 228.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E-04	2.441E-02	25	D014	1 0 0 0 1	

1354. C₈H₆BrNS

4-Bromobenzyl isothiocyanate

p-Bromobenzyl isothiocyanate

RN: 2076-56-4

MP (°C):

MW: 228.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	1.483E-02	25	D014	1 0 0 0 1	
1.500E-04	3.422E-02	25	D019	1 1 1 1 2	

1355. C₈H₆CINS

3-Chlorobenzyl isothiocyanate

m-Chlorobenzyl isothiocyanate

RN: 3694-58-4 MP (°C):

MW: 183.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	2.516E-02	25	D014	1 0 0 0 1	

1356. C₈H₆CINS

4-Chlorobenzyl isothiocyanate

p-Chlorobenzyl isothiocyanate

RN: 3694-45-9 MP (°C):

MW: 183.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-04	2.718E-02	25	D014	1 0 0 0 1	

1357. C₈H₆Cl₂O₃

2,4-Dichlorophenoxyacetic acid

2,4-D

(2,4-Dichlorophenoxy)acetic acid

RN: 94-75-7 MP (°C): 138

MW: 221.04 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.805E-03	6.200E-01	20	F311	1 2 2 2 1	
2.443E-03	5.400E-01	20	M061	1 0 0 0 2	
2.939E-03	6.496E-01	21.50	B200	1 0 0 0 0	
4.072E-03	9.000E-01	22.5	G301	0 0 0 0 0	
3.060E-03	6.764E-01	24.99	N417	0 0 0 0 0	
3.085E-03	6.820E-01	25	B164	1 0 1 1 2	
3.280E-03	7.250E-01	25	B185	0 0 0 0 0	
4.026E-03	8.900E-01	25	F071	1 1 2 1 2	
2.360E-03	5.217E-01	25	L030	1 0 2 1 2	
2.805E-03	6.200E-01	25	M161	1 0 0 0 2	
2.713E-03	5.996E-01	ns	B100	0 0 0 0 0	
4.072E-03	9.000E-01	ns	B185	0 0 0 0 0	
1.810E-03	4.000E-01	ns	B185	0 0 0 0 0	
2.500E-03	5.526E-01	ns	F184	0 0 0 0 1	
4.072E-03	9.000E-01	ns	K138	0 0 0 0 1	
2.805E-03	6.200E-01	ns	L024	0 0 0 0 2	
4.298E-03	9.500E-01	ns	M110	0 0 0 0 0	EFG
1.259E-03	2.783E-01	ns	M163	0 0 0 0 0	EFG
4.026E-03	8.900E-01	ns	M344	0 0 0 0 2	
2.488E-03	5.500E-01	ns	N013	0 0 0 0 2	

1358. C₈H₆Cl₂O₃

Dicamba

2-Methoxy-3,6-dichlorobenzoic acid

RN: 1918-00-9 **MP (°C):** 98
MW: 221.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.036E-02	4.500E+00	25	B200	1 0 0 0 1	
2.036E-02	4.500E+00	25	M161	1 0 0 0 1	
3.591E-02	7.937E+00	ns	B100	0 0 0 0 0	

1359. C₈H₆Cl₂O₃

3,5-Dichlorophenoxyacetic acid

3,5-D

RN: 587-64-4 **MP (°C):**
MW: 221.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.350E-03	9.615E-01	25	L030	1 0 2 1 2	

1360. C₈H₆Cl₂O₃

3,4-Dichlorophenoxyacetic acid

3,4-D

RN: 588-22-7 **MP (°C):** 138
MW: 221.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.070E-03	4.576E-01	25	L030	1 0 2 1 2	
2.090E-03	4.620E-01	ns	B185	0 0 0 0 0	

1361. C₈H₆Cl₂O₃

2,6-Dichlorophenoxyacetic acid

2,6-D

RN: 575-90-6 **MP (°C):**
MW: 221.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.050E-03	1.558E+00	25	L030	1 0 2 1 2	

1362. C₈H₆Cl₂O₃

2,3-Dichlorophenoxyacetic acid

2,3-D

RN: 2976-74-1 **MP (°C):** 173
MW: 221.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-03	3.426E-01	25	L030	1 0 2 1 2	

1363. C₈H₆Cl₂O₃

2,5-Dichlorophenoxyacetic acid

2,5-D

RN: 582-54-7 **MP (°C):**
MW: 221.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.420E-03	5.349E-01	25	L030	1 0 2 1 2	

1364. C₈H₆Cl₄O₂

Tetrachloroveratrole

3,4,5,6-Tetrachloro-1,2-dimethoxybenzene

RN: 944-61-6 **MP (°C):**
MW: 275.95 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.762E-06	1.590E-03	25	L348	1 2 2 1 2	

1365. C₈H₆Cl₅NO₂

Penclomedine

Pyridine

3,5-Dichloro-2,4-dimethoxy-6-(trichloromethyl)

NSC 338720

RN: 108030-77-9 **MP (°C):**
MW: 325.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.229E-06	4.000E-04	25	P325	0 0 0 0 0	
1.229E-06	4.000E-04	25	P336	0 0 0 0 0	

1366. C₈H₆F₃N₃O₄S₂

Flumethiazide

6-(Trifluoromethyl)-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide

6-Trifluoromethyl-7-sulfamoyl-4H-1,2,4-benzothiadiazine 1,1-dioxide

Trifluoromethylthiazide

RN: 148-56-1 **MP (°C):****MW:** 329.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.189E-03	1.050E+00	rt	A095	0 0 2 2 2	

1367. C₈H₆INS

3-Iodobenzyl isothiocyanate

m-Iodobenzyl isothiocyanate**RN:** 3696-68-2 **MP (°C):****MW:** 275.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-05	1.513E-02	25	D014	1 0 0 0 1	

1368. C₈H₆INS

4-Iodobenzyl isothiocyanate

p-Iodobenzyl isothiocyanate**RN:** 3694-49-3 **MP (°C):****MW:** 275.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.100E-05	1.403E-02	25	D014	1 0 0 0 1	

1369. C₈H₆N₂O₂S

3-Nitrobenzyl isothiocyanate

m-Nitrobenzyl isothiocyanate**RN:** 3696-69-3 **MP (°C):****MW:** 194.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.593E-02	25	D014	1 0 0 0 1	

1370. C₈H₆N₂O₂S

4-Nitrobenzyl isothiocyanate

p-Nitrobenzyl isothiocyanate**RN:** 3694-47-1 **MP (°C):****MW:** 194.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.330E-04	4.525E-02	25	D014	1 0 0 0 1	

1371. C₈H₆N₄O₅

Nitrofurantoin

1-[(5-Nitrofurfurylidene)amino]hydantoin

Furatoin

Macrodantin

Macrobid

Welfurin

RN: 67-20-9**MP (°C):** 268**MW:** 238.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.619E-04	1.100E-01	22	B154	1 1 1 1 1	pH 3.5
3.338E-04	7.950E-02	24	C034	2 0 2 2 2	
3.338E-04	7.950E-02	24	C118	1 0 0 0 2	
5.207E-04	1.240E-01	25	M457	0 0 0 0 0	
4.753E-04	1.132E-01	30	C011	2 0 2 1 0	EFG
4.761E-04	1.134E-01	30	C034	2 0 2 2 2	
4.761E-04	1.134E-01	30	C118	1 0 0 0 2	
8.264E-04	1.968E-01	37	A330	0 0 0 0 0	
1.142E-03	2.720E-01	37	B044	2 2 2 1 2	pH 7.2
7.310E-04	1.741E-01	37	C011	2 0 2 1 0	EFG
7.310E-04	1.741E-01	37	C034	2 0 2 2 2	
7.310E-04	1.741E-01	37	C118	1 0 0 0 2	
5.878E-04	1.400E-01	37	E044	1 0 1 1 2	
6.508E-04	1.550E-01	37	P034	1 0 0 0 2	pH 5
1.055E-03	2.512E-01	45	C034	2 0 2 2 2	
1.055E-03	2.512E-01	45	C118	1 0 0 0 2	
7.978E-04	1.900E-01	ns	K444	0 0 0 0 0	
5.249E-04	1.250E-01	ns	P033	0 0 0 0 2	
5.248E-04	1.250E-01	ns	R427	0 0 0 0 0	

1372. C₈H₆N₄O₈

Alloxanthin

Uroxine

Alloxanthin hydrate

RN: 76-24-4**MP (°C):** 254dec**MW:** 286.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-03	5.017E-01	25	B119	1 0 2 2 0	EFG
1.013E-02	2.900E+00	25	F300	1 0 0 0 1	
2.097E-01	6.000E+01	100	F300	1 0 0 0 0	

1373. C₈H₆N₄S₂

Methylthiobenzothiazole

Benzothiazole

RN: 76006-86-5 **MP (°C):**
MW: 222.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-04	1.100E-01	22	P323	0 0 0 0 0	

1374. C₈H₆O₂

Phthalic dicarboxaldehyde

o-Phthalaldehyd

RN: 643-79-8 **MP (°C):** 56.5
MW: 134.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-01	1.400E+01	h	F300	0 0 0 0 1	

1375. C₈H₆O₂

Terephthalidicarboxaldehyde

Terephthalaldehyd

RN: 623-27-8 **MP (°C):** 115
MW: 134.14 **BP (°C):** 246.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.491E-03	2.000E-01	20	F300	1 0 0 0 0	
1.297E-01	1.740E+01	100	F300	1 0 0 0 1	

1376. C₈H₆O₃

Piperonal

Heliotropine

3,4-Dihydroxybenzaldehyde methylene ketal

Methylenedioxy procatechuic aldehyde

Protocatechuic aldehyde methylene ether

Piperonyl aldehyde

RN: 120-57-0 **MP (°C):** 37
MW: 150.14 **BP (°C):** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.331E-02	3.500E+00	20	F300	1 0 0 0 1	
4.463E-02	6.700E+00	78	F300	1 0 0 0 1	

1377. C₈H₆O₃

Benzoylformic acid

Phenyglyoxilic acid

RN: 611-73-4

MP (°C): 67

MW: 150.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.128E+00	9.200E+02	0	C020	1 2 1 1 1	

1378. C₈H₆O₄

1,4-Benzenedicarboxylic acid

Terephthalic acid

p-Phthalic acid

RN: 100-21-0

MP (°C):

MW: 166.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.029E-05	1.500E-02	20	F300	1 0 0 0 1	
1.920E-03	3.190E-01	25	C316	0 0 0 0 0	0.1M HCL
6.019E-04	9.999E-02	80	A027	1 0 0 0 0	

1379. C₈H₆O₄

1,2-Benzenedicarboxylic acid

o-Phthalic acid

Phthalic acid

Phthalsaeure

Benzene-1,2-dicarboxylic acid

RN: 88-99-3

MP (°C): 230

MW: 166.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-02	2.295E+00	0	M043	1 0 0 0 1	
2.219E-02	3.686E+00	2	A027	1 0 0 0 1	
2.159E-02	3.587E+00	10	M043	1 0 0 0 1	
7.935E-03	1.318E+00	10	S198	2 1 2 2 2	
1.571E-02	2.611E+00	10.49	A341	0 0 0 0 0	
3.471E-02	5.767E+00	20	A027	1 0 0 0 1	
3.435E-02	5.707E+00	20	F069	2 2 2 2 2	
3.431E-02	5.700E+00	20	F300	1 0 0 0 1	
3.352E-02	5.569E+00	20	M043	1 0 0 0 1	
7.214E-03	1.199E+00	20	S198	2 1 2 2 2	
3.915E-02	6.504E+00	22.99	A341	0 0 0 0 0	
4.200E-02	6.978E+00	24.99	A341	0 0 0 0 0	
8.600E-02	1.429E+01	25	H084	1 0 0 0 1	
8.520E-02	1.415E+01	25	K040	1 0 2 1 2	
4.192E-02	6.965E+00	25	M030	2 1 0 1 2	
4.279E-02	7.109E+00	25.8	W029	1 2 1 1 2	
4.808E-02	7.988E+00	28	D050	1 2 1 2 2	
5.152E-02	8.560E+00	29.49	A341	0 0 0 0 0	

(continued)

1379. C₈H₆O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-02	8.141E+00	30	H019	0 0 0 0 0	
4.777E-02	7.937E+00	30	M043	1 0 0 0 0	
8.235E-03	1.368E+00	30	S198	2 1 2 2 2	
5.865E-02	9.743E+00	33.99	A341	0 0 0 0 0	
6.033E-02	1.002E+01	35	M030	2 1 0 1 2	
6.561E-02	1.090E+01	35.99	A341	0 0 0 0 0	
6.925E-02	1.150E+01	37.99	A341	0 0 0 0 0	
7.137E-02	1.186E+01	40	M043	1 0 0 0 1	
8.274E-02	1.375E+01	41.99	A341	0 0 0 0 0	
7.865E-02	1.307E+01	43.7	W029	1 2 1 1 2	
8.981E-02	1.492E+01	43.99	A341	0 0 0 0 0	
8.991E-02	1.494E+01	44.99	A341	0 0 0 0 0	
8.580E-02	1.425E+01	45	M030	2 1 0 1 2	
9.890E-02	1.643E+01	45.99	A341	0 0 0 0 0	
9.753E-02	1.620E+01	48.9	W029	1 2 1 1 2	
1.212E-01	2.014E+01	49.99	A341	0 0 0 0 0	
1.116E-01	1.854E+01	49.99	A341	0 0 0 0 0	
1.349E-01	2.241E+01	53.99	A341	0 0 0 0 0	
1.277E-01	2.122E+01	55	M030	2 1 0 1 2	
1.339E-01	2.225E+01	58.0	W029	1 2 1 1 2	
1.639E-01	2.724E+01	60	M043	1 0 0 0 1	
1.741E-01	2.892E+01	60.99	A341	0 0 0 0 0	
1.695E-01	2.815E+01	63.7	W029	1 2 1 1 2	
2.145E-01	3.564E+01	64.99	A341	0 0 0 0 0	
1.892E-01	3.144E+01	65	M030	2 1 0 1 2	
2.826E-01	4.695E+01	75	M030	2 1 0 1 2	
3.042E-01	5.053E+01	77.8	W029	1 2 1 1 2	
3.567E-01	5.927E+01	80	M043	1 0 0 0 1	
4.334E-01	7.200E+01	85	F300	1 0 0 0 0	
4.297E-01	7.138E+01	85	M030	2 1 0 1 2	
4.248E-01	7.058E+01	85.7	W029	1 2 1 1 2	
6.377E-01	1.059E+02	94.8	W029	1 2 1 1 2	
9.182E-01	1.525E+02	100	M043	1 0 0 0 2	
8.208E-01	1.364E+02	101.1	W029	1 2 1 1 2	
1.370E+00	2.276E+02	113.8	W029	1 2 1 1 2	
9.015E-03	1.498E+00	ns	F014	0 0 0 0 2	
2.458E-02	4.083E+00	rt	H431	0 0 0 0 0	

1380. C₈H₆O₄

Isophthalic acid

1,3-Benzenedicarboxylic acid

m-Phthalic acid

RN: 121-91-5 MP (°C): 345

MW: 166.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.611E-04	6.000E-02	2	A027	1 0 0 0 0	
6.019E-04	9.999E-02	20	A027	1 0 0 0 0	

(continued)

1380. C₈H₆O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-03	1.811E-01	28.29	L437	0 0 0 0 0	
1.656E-03	2.752E-01	40.99	L437	0 0 0 0 0	
2.535E-03	4.212E-01	51.99	L437	0 0 0 0 0	
4.021E-03	6.681E-01	64.99	L437	0 0 0 0 0	
6.260E-03	1.040E+00	76.49	L437	0 0 0 0 0	
6.013E-03	9.990E-01	80	A027	1 0 0 0 0	
8.300E-03	1.379E+00	83.49	L437	0 0 0 0 0	
9.441E-03	1.568E+00	86.47	L437	0 0 0 0 0	
1.286E-02	2.137E+00	93.42	L437	0 0 0 0 0	
4.610E-04	7.659E-02	rt	H431	0 0 0 0 0	

1381. C₈H₆O₅

2-Hydroxyisophthalic acid

2-Hydroxy-*iso*-phthalsaeure

RN: 606-19-9 MP (°C): 244
 MW: 182.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E-01	2.640E+01	100	F300	1 0 0 0 2	

1382. C₈H₆O₅

4-Hydroxyisophthalic acid

4-Hydroxy-*iso*-phthasaeure

RN: 636-46-4 MP (°C): 310
 MW: 182.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.647E-03	3.000E-01	24	F300	1 0 0 0 1	

1383. C₈H₆O₅

5-Hydroxyisophthalic acid

5-Hydroxy-*iso*-phthalsaeure

RN: 618-83-7 MP (°C): 293
 MW: 182.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.294E-03	6.000E-01	15	F300	1 0 0 0 1	
8.889E-01	1.619E+02	99	F300	1 0 0 0 2	

1384. C₈H₆S

Thianaphthene
 Benzo[b]thiophene
 Benzothiofuran
 1-Benzothiophene
RN: 95-15-8 **MP (°C):** 29–32
MW: 134.20 **BP (°C):** 221–222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-03	2.162E-01	59.0	L339	2 0 2 2 2	
2.610E-03	3.503E-01	78.5	L339	2 0 2 2 2	
4.386E-03	5.886E-01	99.0	L339	2 0 2 2 2	

1385. C₈H₇BrN₂O₃

o-Nitro-*o*-bromacetanilide
 2-Bromo-5-nitroacetanilide
RN: 245115-83-7 **MP (°C):**
MW: 259.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.720E-02	2.000E+01	rt	F043	0 0 2 1 1	

1386. C₈H₇BrN₂O₃

p-Nitro-*o*-bromacetanilide
 2-Bromo-4-nitroacetanilide
RN: 57045-86-0 **MP (°C):**
MW: 259.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.832E-02	1.770E+01	rt	F043	0 0 2 1 2	

1387. C₈H₇ClN₂O₃

p-Nitro-*o*-chloracetanilide
 2-Chloro-4-nitroacetanilide
RN: 881-87-8 **MP (°C):**
MW: 214.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.172E-02	1.110E+01	rt	F043	0 0 2 1 2	

1388. C₈H₇CIN₂O₃*o*-Nitro-*o*-chloracetanilide

2-Chloro-5-nitroacetanilide

RN: 72487-80-0 MP (°C):

MW: 214.61 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.172E-02	1.110E+01	rt	F043	0 0 2 1 2	

1389. C₈H₇ClO₃

4-Chlorophenoxyacetic acid

4-CPA

p-Chlorophenoxyacetic acid

RN: 122-88-3 MP (°C): 157

MW: 186.60 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.545E-03	8.480E-01	25	B164	1 0 1 1 2	
2.042E-03	3.810E-01	25	B185	0 0 0 0 0	
5.130E-03	9.572E-01	25	L030	1 0 2 1 2	

1390. C₈H₇ClO₃

3-Chlorophenoxyacetic acid

m-Chlorophenoxyacetic acid

RN: 588-32-9 MP (°C):

MW: 186.60 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.265E-02	2.360E+00	25	L030	1 0 2 1 2	

1391. C₈H₇ClO₃

2-Chlorophenoxyacetic acid

o-Chlorophenoxyacetic acid

RN: 614-61-9 MP (°C): 146

MW: 186.60 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.850E-03	1.278E+00	25	L030	1 0 2 1 2	

1392. C₈H₇Cl₂NO₂

Chloramben methyl ester

Vegiben 2E

Methyl 3-amino-2,5-dichlorobenzoate

Amchem 65-81-B

Methyl chloramben

Chloramben methyl

RN: 7286-84-2 **MP (°C):** 63.5**MW:** 220.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.453E-04	1.200E-01	20	M161	1 0 0 0 2	

1393. C₈H₇Cl₃O

2,4,6-Trichloro-3,5-dimethyl-phenol

3,5-Xylenol, 2,4,6-trichloro-

RN: 6972-47-0 **MP (°C):****MW:** 225.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-05	4.961E-03	25	B316	0 0 0 0 0	

1394. C₈H₇Cl₃O₂

3,4,5-Trichloroveratrole

4,5,6-Trichloroveratrole

RN: 16766-29-3 **MP (°C):** 66**MW:** 241.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.265E-05	1.030E-02	25	L348	1 2 2 1 2	

1395. C₈H₇N

Indole

2,3-Benzopyrrole

Benzopyrrole

1-Benzazole

1-Benzol β pyrrol**RN:** 120-72-9 **MP (°C):** 52**MW:** 117.15 **BP (°C):** 253

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.219E-02	1.080E+01	25	K119	1 0 0 0 2	
3.037E-02	3.558E+00	25	P051	2 1 1 2 2	
3.037E-02	3.558E+00	25.00	P007	2 1 2 2 2	

1396. C₈H₇N*p*-Toluonitrile*p*-Cyanotoluene*p*-Methylbenzonitrile

4-Methylbenzenecarbonitrile

RN: 104-85-8**MP (°C):****MW:** 117.15**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	1.523E+00	25	M327	1 0 0 1 2	

1397. C₈H₇NOS*m*-Methoxyphenyl isothiocyanate*3*-Methoxyphenyl isothiocyanate**RN:** 3125-64-2**MP (°C):****MW:** 165.22**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	4.461E-02	25	K032	2 2 0 1 2	

1398. C₈H₇NOS*p*-Methoxyphenyl isothiocyanate*4*-Methoxyphenylisothiocyanate**RN:** 2284-20-0**MP (°C):** 18.0**MW:** 165.22**BP (°C):** 280.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-04	4.130E-02	25	D019	1 1 1 1 2	

1399. C₈H₇NO₃

Oxanilic acid

N-Phenylxallic acid monoamide

Oxanilsaure

RN: 500-72-1**MP (°C):** 150**MW:** 165.15**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.990E-02	8.241E+00	25	D058	1 0 1 1 2	

1400. C₈H₇NO₄

6-Nitro-3-methylbenzoic acid

2-Nitro-5-methylbenzoic acid

5-Methyl-2-nitrobenzoic acid

3-Methyl-6-nitrobenzoic acid

RN: 3113-72-2 **MP (°C):****MW:** 181.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.043E-02	3.700E+00	10	G063	1 0 0 0 1	
2.595E-02	4.700E+00	20	G063	1 0 0 0 1	
9.385E-02	1.700E+01	40	G063	1 0 0 0 1	
9.937E-02	1.800E+01	50	G063	1 0 0 0 1	
1.490E-01	2.700E+01	60	G063	1 0 0 0 1	
1.932E-01	3.500E+01	65	G063	1 0 0 0 1	
2.484E-01	4.500E+01	70	G063	1 0 0 0 1	
3.643E-01	6.600E+01	80	G063	1 0 0 0 1	
3.699E-01	6.700E+01	100	G063	1 0 0 0 1	

1401. C₈H₇NO₄

2-Nitro-3-methylbenzoic acid

2-Nitro-*m*-toluic acid

3-Methyl-2-nitrobenzoic acid

RN: 5437-38-7 **MP (°C):****MW:** 181.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.208E-03	4.000E-01	20	G063	1 0 0 0 1	
8.832E-03	1.600E+00	40	G063	1 0 0 0 1	
3.202E-02	5.800E+00	80	G063	1 0 0 0 1	
3.312E-02	6.000E+00	100	G063	1 0 0 0 0	

1402. C₈H₇NS

Benzyl isothiocyanate

Benzylisothiocyanate

Isothiocyanatomethylbenzene

RN: 622-78-6 **MP (°C):** 112**MW:** 149.22 **BP (°C):** 242

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-04	1.089E-01	25	D014	1 0 0 0 2	

1403. C₈H₇NS

p-Tolyl isothiocyanate
4-Tolylisothiocyanate

RN: 622-59-3 **MP (°C):** 25
MW: 149.22 **BP (°C):** 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-05	2.835E-03	25	D019	1 1 1 1 1	

1404. C₈H₇NS

m-Methylphenyl isothiocyanate
3-Methylphenyl isothiocyanate

RN: 614-69-7 **MP (°C):**
MW: 149.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-04	2.119E-02	25	K032	2 2 0 1 2	

1405. C₈H₇N₅O

7-Acetamidopteridine

RN: **MP (°C):**
MW: 189.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.035E-02	7.634E+00	100	A083	1 2 0 0 0	

1406. C₈H₇N₅O

2-Acetamidopteridine

RN: **MP (°C):**
MW: 189.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-01	3.226E+01	100	A083	1 2 0 0 0	

1407. C₈H₇N₅O

4-Acetamidopteridine

RN: **MP (°C):**
MW: 189.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.762E+00	3.333E+02	100	A083	1 2 0 0 0	

1408. C₈H₇N₅O₈

2,4,6-Trinitrophenylethylnitramine

Tetreethyl

Trinitrophenylethylnitramine

Ethyl tetryl

RN: 6052-13-7 MP (°C):

MW: 301.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E-04	6.000E-02	22	D067	1 2 0 0 0	
8.633E-04	2.600E-01	50	D067	1 2 0 0 1	
8.998E-03	2.710E+00	100	D067	1 2 0 0 2	

1409. C₈H₈

Styrene

Phenylethylene

Styrolene

Styrol

Ethenylbenzene

Annamene

RN: 100-42-5 MP (°C): -30

MW: 104.15 BP (°C): 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.784E-03	2.899E-01	7	L028	1 0 1 1 1	
2.400E-03	2.499E-01	15	L028	1 0 1 1 1	
1.152E-03	1.200E-01	20	L096	1 2 0 2 2	
3.167E-03	3.299E-01	24	L028	1 0 1 1 1	
2.880E-03	3.000E-01	25	A002	1 2 1 1 1	
1.540E-03	1.604E-01	25	B173	2 0 2 2 2	
2.975E-03	3.099E-01	25	L028	1 0 1 1 1	
3.455E-03	3.599E-01	32	L028	1 0 1 1 1	
3.839E-03	3.998E-01	40	L028	1 0 1 1 1	
3.839E-03	3.998E-01	44	L028	1 0 1 1 1	
4.319E-03	4.498E-01	49	L028	1 0 1 1 1	
4.319E-03	4.498E-01	51	L028	1 0 1 1 1	
4.798E-03	4.998E-01	56	L028	1 0 1 1 1	
8.658E-02	9.018E+00	65	A324	2 2 2 1 1	
5.566E-03	5.797E-01	65	L028	1 0 1 1 1	

1410. C₈H₈BrCl₂O₃PS

Bromophos

O-(4-Bromo-2,5-dichlorophenyl) *O,O*-dimethyl phosphorothioate

Nexion

Brofene

Brophene

Omexan

RN: 2104-96-3 **MP (°C):** 51**MW:** 366.00 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.557E-07	2.400E-04	10	B324	0 0 0 0 0	
6.558E-07	2.400E-04	10	B324	0 0 0 0 0	
8.197E-07	3.000E-04	20	B169	2 1 1 1 1	<i>sic</i>
9.290E-07	3.400E-04	20	B324	0 0 0 0 0	
9.290E-07	3.400E-04	20	B324	0 0 0 0 0	
2.732E-06	1.000E-03	20	F311	1 2 2 2 1	<i>sic</i>
1.093E-04	4.000E-02	20	M061	1 0 0 0 1	
1.093E-04	4.000E-02	20	W311	1 0 0 0 1	
2.634E-06	9.641E-04	30	B324	0 0 0 0 0	
2.623E-06	9.600E-04	30	B324	0 0 0 0 0	
1.093E-04	4.000E-02	ns	E050	0 0 0 0 1	
1.093E-04	4.000E-02	rt	M161	0 0 0 0 1	

1411. C₈H₈BrNO

4'-Bromoacetanilide

Acetamide, *N*-(4-bromophenyl)-

Acetanilide, 4'-bromo-

Bromoantifebrin

RN: 103-88-8 **MP (°C):****MW:** 214.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	1.498E-01	25	D044	0 0 0 0 0	

1412. C₈H₈ClNO*p*-ChloroacetanilideAcetamide, *N*-(4-chlorophenyl)-

Acetanilide, 4'-chloro-

RN: 539-03-7 **MP (°C):****MW:** 169.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.696E-01	25	D044	0 0 0 0 0	

1413. C₈H₈Cl₂IO₃PS

Iodofenphos

O-(2,5-Dichloro-4-iodophenyl) *O,O*-dimethyl phosphorothioate

Nuvanol-N

Dimethyl *O*-2,5-dichloro-4-iodophenyl thiophosphate

Alfacron

Jodfenphos

RN: 18181-70-9 MP (°C): 72

MW: 413.00 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.421E-07	1.000E-04	20	B169	2 1 1 1 1	
4.843E-06	2.000E-03	20	M161	1 0 0 0 0	

1414. C₈H₈Cl₂O

2,4-Dichloro-6-ethyl-phenol

Phenol, 2,4-dichloro-6-ethyl-

RN: 24539-94-4 MP (°C):

MW: 191.06 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	2.484E-01	25	B316	0 0 0 0 0	

1415. C₈H₈Cl₂O₂

Chloroneb

Demosan

Terraneb

Terraneb SP

1,4-Dichloro-2,5-dimethoxybenzene

Terraneb B

RN: 2675-77-6 MP (°C): 134.5

MW: 207.06 BP (°C): 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.864E-05	8.000E-03	25	M161	1 0 0 0 0	

1416. C₈H₈Cl₂O₂

4,5-Dichloroveratrole

Benzene, 1,2-dichloro-4,5-dimethoxy-

RN: 2772-46-5 MP (°C): 83

MW: 207.06 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.492E-04	7.230E-02	25	L348	1 2 2 1 2	average of 2

1417. C₈H₈Cl₃O₃PS

Ronnel

Fenchlorphos

Dermafos

Dimethyl trichlorophenylthiophosphate

RN: 299-84-3 MP (°C): 35

MW: 321.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.866E-06	6.000E-04	20	B169	2 2 1 1 1	
3.359E-06	1.080E-03	20	C053	0 0 0 0 0	
3.110E-06	1.000E-03	20	E048	1 2 1 1 0	
7.775E-06	2.500E-03	20	F311	1 2 2 2 1	
5.287E-06	1.700E-03	ns	F040	1 2 2 2 1	
3.359E-06	1.080E-03	ns	F071	0 1 2 1 2	
1.866E-05	6.000E-03	ns	K138	0 0 0 0 1	
1.368E-04	4.400E-02	ns	M061	0 0 0 0 1	
1.244E-04	4.000E-02	rt	M161	0 0 0 0 1	

1418. C₈H₈FNO

4'-Fluoroacetanilide

Acetamide, N-(4-fluorophenyl)-

4-Fluoroacetanilide

RN: 351-83-7 MP (°C):

MW: 153.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.630E-02	2.496E+00	25	D044	0 0 0 0 0	

1419. C₈H₈F₃N₃O₄S₂

Hydroflumethiazide

Diucardin

Saluron

RN: 135-09-1 MP (°C): 272

MW: 331.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.449E-03	4.800E-01	37	C087	0 0 0 0 0	
2.048E-03	6.785E-01	37	C315	0 0 0 0 0	0.1N HCL, average of 4
5.643E-04	1.870E-01	ns	B404	0 2 1 1 0	
9.958E-04	3.299E-01	rt	K144	0 0 0 0 1	

1420. C₈H₈INO*p*-Iodoaniline-*N*-acetate4-Iodanilin-*N*-acetat

4-Iodoacetanilide

Acetanilide, 4'-iodo-

4-Acetamidophenyl iodide

p-Iodoacetanilide

RN: 622-50-4 MP (°C):

MW: 261.06 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	1.827E-01	25	D044	0 0 0 0 0	

1421. C₈H₈N₂O₂

Phthalamide

1,2-Benzenedicarboxamide

RN: 88-96-0 MP (°C): 228

MW: 164.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.218E-03	2.000E-01	20	A027	1 0 0 0 0	
3.594E-02	5.900E+00	30	K004	1 0 0 0 1	sic

1422. C₈H₈N₂O₂

Ricinine

Ricinin

RN: 524-40-3 MP (°C): 201.5

MW: 164.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.645E-02	2.700E+00	10	F300	1 0 0 0 1	

1423. C₈H₈N₂O₃4-Nitroaniline-*N*-acetate4-Nitro-anilin-*N*-acetat*p*-Nitroacetanilide

1-Nitro-4-acetylaminobenzene

RN: 104-04-1 MP (°C): 216

MW: 180.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.200E+00	20	F300	1 0 0 0 1	
6.000E-04	1.081E-01	25	D044	0 0 0 0 0	
1.221E-02	2.200E+00	rt	F043	0 0 2 1 1	

1424. C₈H₈N₂O₃2-Nitroaniline-*N*-acetate2-Nitro-anilin-*N*-acetat*o*-Nitroacetanilide**RN:** 552-32-9 **MP (°C):****MW:** 180.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.200E+00	20	F300	1 0 0 0 1	
1.221E-02	2.200E+00	rt	F043	0 0 2 1 1	

1425. C₈H₈N₂O₆S

MB 8882

Methyl *N*-(4-nitrobenzenesulphonyl)carbamate**RN:** 3337-70-0 **MP (°C):** 151**MW:** 260.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.839E-03	9.990E-01	ns	M061	0 0 0 0 0	

1426. C₈H₈N₄

6,7-Dimethylpteridine

6,7-Dimethylpteridine

RN: 704-61-0 **MP (°C):****MW:** 160.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.468E-01	5.556E+01	20	A083	1 2 0 0 0	

1427. C₈H₈N₄

Hydralazine

Apresoline

RN: 86-54-4 **MP (°C):** 172**MW:** 160.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.996E-05	4.800E-03	22.5	B440	0 0 0 0 0	

1428. C₈H₈N₄O

4-Hydroxy-6,7-dimethylpteridine

4-Hydroxy-6,7-dimethylpteridine

RN: 14684-54-9 MP (°C):

MW: 176.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.155E-03	9.083E-01	22.5	A085	1 2 0 0 0	

1429. C₈H₈N₄O₂

H-Pyrazolo[3,4-d]pyrimidin-4-one, 1,5-dihydro-1-(1-oxopropyl)-

RN: 96448-61-2 MP (°C):

MW: 192.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.561E-03	3.000E-01	22	B428	1 2 1 2 1	

1430. C₈H₈N₄O₂S₂

2-Sulfanilamido-1,3,4-thiadiazole

Sulfathiadiazole

Sulfanilamide, N1-1,3,4-thiadiazol-2-yl-

RN: 16806-29-4 MP (°C):

MW: 256.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.848E-03	7.300E-01	37	R045	1 2 1 1 1	

1431. C₈H₈N₄O₃

1-Acetoxyethyl allopurinol

4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[(acetyloxy)methyl]-1,5-dihydro-

RN: 98846-64-1 MP (°C): 257-258

MW: 208.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-03	5.800E-01	22	B322	0 0 0 0 0	

1432. C₈H₈N₄O₄

Nifuradene

1-[5-Nitrofuryllidene)amino]-2-imidazolidinone

RN: 555-84-0 MP (°C): 261.5

MW: 224.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-04	8.800E-02	ns	I310	0 0 0 0 0	

1433. C₈H₈N₄O₄S₃

CL 11366

RN:**MW:** 320.37**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.405E-03	4.500E-01	ns	M032	0 0 0 0 1	

1434. C₈H₈N₄O₄S₃

Benzolamide

2-Benzenesulfonamide-1,3,4-thiadiazole-5-sulfonamide

5-Benzenesulfonamido-1,3,4-thiadiazole-2-sulfonamide

1,3,4-Thiadiazole-2-sulfonamide, 5-[(phenylsulfonyl)amino]-

1,3,4-Thiadiazole-2-sulfonamide, 5-benzenesulfonamido-

RN: 3368-13-6 **MP (°C):****MW:** 320.37 **BP (°C):** 585.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.844E-01	25	C415	1 0 0 1 0	

1435. C₈H₈N₄O₆

2,4,6-Trinitroethylaniline

2-4-6-Trinitromonoethylaniline

RN: 7449-27-6 **MP (°C):****MW:** 256.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.904E-04	1.000E-01	19	D067	1 2 0 0 2	
1.210E-03	3.100E-01	50	D067	1 2 0 0 2	
5.699E-03	1.460E+00	100	D067	1 2 0 0 2	

1436. C₈H₈O

Acetophenone

Acetophenon

Methyl phenyl ketone

RN: 98-86-2 **MP (°C):** 20.05**MW:** 120.15 **BP (°C):** 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.503E-02	5.411E+00	24	H106	1 0 2 2 2	
4.611E-02	5.540E+00	24	M303	1 0 1 1 2	
5.243E-02	6.300E+00	25	A003	1 2 1 2 2	
4.470E-02	5.371E+00	25	B019	1 0 1 2 0	
4.470E-02	5.371E+00	25	B092	2 1 1 1 1	
9.600E-02	1.153E+01	25	D407	1 0 2 2 2	
5.600E-03	6.729E-01	25	F063	1 1 0 0 1	
6.605E-02	7.937E+00	60	B092	2 1 1 1 1	

1437. C₈H₈O

Styrene oxide

1,2-Epoxyethylbenzene

RN: 96-09-3 **MP (°C):** -36.8
MW: 120.15 **BP (°C):** 194.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.324E-02	2.792E+00	25	I313	0 0 0 0 0	

1438. C₈H₈O

2,2,3-Trimethyl-3-pentanol

2,2,3-Trimethylpentanol-3

RN: 7294-05-5 **MP (°C):** -6
MW: 120.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.120E+00	4.950E+02	20	G007	1 2 0 1 2	
4.119E+00	4.949E+02	25	G007	1 2 0 1 2	
4.119E+00	4.949E+02	30	G007	1 2 0 1 2	

1439. C₈H₈O

4-Methylbenzaldehyde

p-Methylbenzaldehyde

RN: 104-87-0 **MP (°C):**
MW: 120.15 **BP (°C):** 204

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.890E-02	2.271E+00	25	M017	1 2 0 1 2	

1440. C₈H₈O₂

2'-Hydroxyacetophenone

1-(2-Hydroxyphenyl)ethanone

2-Acetylphenol

RN: 118-93-4 **MP (°C):** 6
MW: 136.15 **BP (°C):** 213 at 717 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-02	6.808E+00	30	K441	0 0 0 0 0	
1.100E-01	1.498E+01	40	K441	0 0 0 0 0	
1.400E-01	1.906E+01	50	K441	0 0 0 0 0	

1441. C₈H₈O₂

4-Hydroxyacetophenone

4'-Hydroxy-acetophenon

RN: 99-93-4

MP (°C): 110

MW: 136.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.271E-02	9.900E+00	22	F300	1 0 0 0 1	
7.000E-02	9.531E+00	30	K441	0 0 0 0 0	
1.400E-01	1.906E+01	40	K441	0 0 0 0 0	
1.800E-01	2.451E+01	50	K441	0 0 0 0 0	

1442. C₈H₈O₂*p*-Anisaldehyde

Anisaldehyd

p-Methoxybenzaldehyde

RN: 123-11-5

MP (°C): 0

MW: 136.15

BP (°C): 249.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E-02	2.000E+00	20	F300	1 0 0 0 0	
3.900E-02	5.310E+00	25	D407	1 0 2 2 2	
3.150E-02	4.289E+00	25	I019	1 0 1 2 2	

1443. C₈H₈O₂*m*-Toluic acid

3-Methylbenzoic acid

m-Methylbenzoic acid β -Methylbenzoic acid

RN: 99-04-7

MP (°C): 112

MW: 136.15

BP (°C): 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-03	9.803E-01	25	F001	1 0 1 0 2	
7.198E-03	9.800E-01	25	F300	1 0 0 0 2	
7.785E-03	1.060E+00	37	M360	1 2 1 1 2	

1444. C₈H₈O₂*p*-Toluic acid

4-Methylbenzoic acid

Toluenecarboxylic acid

RN: 99-94-5**MP (°C):** 180**MW:** 136.15**BP (°C):** 274

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	3.404E-01	25	F001	1 0 1 0 2	
2.938E-03	4.000E-01	25	F300	1 0 0 0 2	
2.277E-03	3.100E-01	37	M360	1 2 1 1 2	
2.780E-03	3.785E-01	ns	C014	0 0 0 1 2	

1445. C₈H₈O₂*o*-Toluic acid*o*-Tolylsaeure*o*-Toluyllic acid

2-Methylbenzoic acid

RN: 118-90-1**MP (°C):** 107**MW:** 136.15**BP (°C):** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-03	1.185E+00	25	F001	1 0 1 0 2	
8.780E-03	1.195E+00	25	R016	0 0 0 0 0	
1.014E-02	1.380E+00	37	M360	1 2 1 1 2	

1446. C₈H₈O₂

Phenylacetic acid

Phenyllessigsaeure

RN: 103-82-2**MP (°C):** 76.5**MW:** 136.15**BP (°C):** 266

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E-01	1.600E+01	20	F071	1 1 2 1 2	
1.219E-01	1.660E+01	20	H080	1 0 0 0 2	
1.219E-01	1.660E+01	20	M344	1 0 0 0 2	
1.300E-01	1.770E+01	25	F300	1 0 0 0 2	
1.267E-01	1.725E+01	25	H071	2 2 2 1 2	
1.310E-01	1.784E+01	25	K040	1 0 2 1 2	
1.300E-01	1.770E+01	25.00	M135	1 2 1 1 2	0.01N sodium phenylacetate
1.451E-01	1.975E+01	30	D033	2 2 1 2 2	
1.910E-01	2.600E+01	35.00	M135	1 2 1 1 2	
2.113E-01	2.877E+01	40	D033	2 2 1 2 2	
2.880E-01	3.921E+01	41.50	M135	1 2 1 1 2	
2.900E-01	3.948E+01	45.00	M135	1 2 1 1 2	
3.650E-01	4.970E+01	58.40	M135	1 2 1 1 2	

(continued)

1446. C₈H₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.350E-01	5.923E+01	68.80	M135	1 2 1 1 2	
5.130E-01	6.985E+01	76.50	M135	1 2 1 1 2	
6.110E-01	8.319E+01	83.00	M135	1 2 1 1 2	
6.860E-01	9.340E+01	86.70	M135	1 2 1 1 2	
7.712E-01	1.050E+02	100	F300	1 0 0 0 2	
1.259E-01	1.714E+01	ns	R424	0 0 0 0 0	

1447. C₈H₈O₂

Methyl benzoate

Methyl *p*-hydroxybenzoate

RN: 93-58-3 MP (°C): -12
 MW: 136.15 BP (°C): 198

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.337E-03	9.990E-01	15	G040	1 0 2 0 0	
3.085E-02	4.200E+00	22	N317	1 1 2 1 2	
2.926E-02	3.984E+00	25	G040	1 0 2 0 0	
1.447E-02	1.970E+00	25	L086	1 0 1 1 2	
1.497E-02	2.038E+00	25	M334	1 0 1 1 2	
1.777E-02	2.420E+00	30	L012	2 0 2 2 2	
1.796E-02	2.445E+00	30	L086	1 0 1 1 2	
3.654E-02	4.975E+00	35	G040	1 0 2 0 0	
2.221E-02	3.024E+00	35	L086	1 0 1 1 2	
2.723E-02	3.708E+00	40	L086	1 0 1 1 2	

1448. C₈H₈O₂Hg

Phenylmercuric acetate

Ceresan

PMAC

Acetate, phenylmercuric

PMA

RN: 62-38-4 MP (°C): 149
 MW: 336.74 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.335E-02	2.470E+01	20	M061	1 0 0 0 2	
1.389E-02	4.678E+00	ns	B185	0 0 0 0 0	
1.396E-02	4.700E+00	ns	N013	0 0 0 0 2	
1.298E-02	4.370E+00	rt	M161	0 0 0 0 2	

1449. C₈H₈O₃

Methyl salicylate

Salicylsaeure-methyl ester

Methyl hydroxybenzoate

Betula oil

Panalgesic

Betula

RN: 119-36-8 **MP (°C):** -8
MW: 152.15 **BP (°C):** 222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.206E-03	6.400E-01	21	B331	0 0 0 0 0	
4.000E-03	6.086E-01	25	D407	1 0 2 2 2	
1.312E-02	1.996E+00	25	R041	0 0 0 0 0	
4.601E-03	7.000E-01	30	F300	1 0 0 0 0	
6.244E-03	9.500E-01	30	L012	2 0 2 2 1	

1450. C₈H₈O₃

Vanillin

4-Hydroxy-3-methoxybenzaldehyde

3-Methoxy-4-hydroxybenzaldehyde

Methylprotocatechic aldehyde

Vanillic aldehyde

Vanillaldehyde

RN: 121-33-5 **MP (°C):** 82
MW: 152.15 **BP (°C):** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.439E-02	6.754E+00	.2	D073	1 1 2 1 1	
1.972E-02	3.000E+00	4.40	M096	1 1 2 1 1	
3.418E-02	5.200E+00	15.60	M096	1 1 2 1 2	
8.114E-02	1.235E+01	20	D073	1 1 2 1 2	
6.572E-02	1.000E+01	20	F300	1 0 0 0 0	
5.915E-02	9.000E+00	23.90	M096	1 1 2 1 2	
4.800E-02	7.303E+00	25	D407	1 0 2 2 2	
7.240E-02	1.102E+01	25	I019	1 0 1 2 2	
9.713E-02	1.478E+01	30	D073	1 1 2 1 2	
8.500E-02	1.293E+01	30	L069	1 0 1 1 0	EFG
1.697E-01	2.582E+01	40	D073	1 1 2 1 2	
3.010E-01	4.580E+01	50	D073	1 1 2 1 2	
3.160E-01	4.807E+01	60	D073	1 1 2 1 2	
3.286E-01	5.000E+01	80	F300	1 0 0 0 0	

1451. C₈H₈O₃

Methylparaben

Me-paraben

Methyl *p*-hydroxybenzoic acid

Methyl 4-hydroxybenzoate

Methyl paraben

RN: 99-76-3

MP (°C): 131

MW: 152.15

BP (°C): 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.310E-03	1.264E+00	15	B355	0 0 0 0 0	
1.026E-02	1.561E+00	15	M352	1 1 1 1 2	
9.970E-03	1.517E+00	20	B355	0 0 0 0 0	
1.334E-02	2.030E+00	20	H056	1 0 2 1 2	
1.441E-02	2.193E+00	25	A059	1 0 1 1 2	
1.140E-02	1.735E+00	25	B355	0 0 0 0 0	
1.639E-02	2.494E+00	25	D081	1 2 2 1 2	
1.600E-02	2.434E+00	25	D339	0 0 0 0 0	
3.162E-02	4.811E+00	25	F322	2 0 1 1 0	EFG
1.364E-02	2.075E+00	25	L075	1 0 1 1 2	
1.393E-02	2.120E+00	25	L338	1 0 1 1 2	
1.460E-02	2.221E+00	25	M014	2 0 1 1 2	
1.585E-02	2.412E+00	25	M352	1 1 1 1 2	
1.643E-02	2.500E+00	25	O027	1 0 1 0 1	
1.485E-02	2.260E+00	25	P013	0 0 0 0 0	
1.446E-02	2.200E+00	25	P053	1 0 1 1 2	
1.600E-02	2.434E+00	27	B129	2 2 2 2 2	
1.500E-02	2.282E+00	27	G078	2 1 0 1 0	EFG
1.600E-02	2.434E+00	27	P019	1 2 1 1 0	EFG
1.450E-02	2.206E+00	27.0	G067	2 0 1 1 2	
1.828E-02	2.782E+00	30	A059	1 0 1 1 2	
1.564E-02	2.380E+00	30	M325	1 0 0 0 1	
2.275E-02	3.462E+00	35	A059	1 0 1 1 2	
2.550E-02	3.880E+00	37	B171	2 0 1 1 2	
2.268E-02	3.451E+00	39.3	G302	2 2 2 2 0	EFG
2.551E-02	3.882E+00	40	A059	1 0 1 1 2	
3.773E-02	5.740E+00	40	M352	1 1 1 1 2	
4.168E-02	6.341E+00	50	M352	1 1 1 1 2	

1452. C₈H₈O₃

D-Mandelic acid

(R)(-)Mandelic acid

(S)-α-Hydroxybenzeneacetic acid

L-Mandelic acid

(S)-(+)Mandelic acid

RN: 17199-29-0

MP (°C): 132

MW: 152.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.310E-01	8.080E+01	0	A043	1 2 1 1 2	
5.310E-01	8.080E+01	0	L035	1 2 2 1 2	

(continued)

1452. C₈H₈O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.874E-01	1.046E+02	10	A043	1 2 1 1 2	
6.874E-01	1.046E+02	10	L035	1 2 2 1 2	
7.766E-01	1.182E+02	15	A043	1 2 1 1 2	
7.766E-01	1.182E+02	15	L035	1 2 2 1 2	
9.158E-01	1.393E+02	20	A043	1 2 1 1 2	
9.158E-01	1.393E+02	20	L035	1 2 2 1 2	
5.371E-01	8.173E+01	24.5	L035	1 2 2 1 1	
5.371E-01	8.173E+01	24.50	A043	1 2 1 1 1	
1.183E+00	1.800E+02	25	A043	1 2 1 1 2	
6.503E-01	9.894E+01	25	C045	2 2 0 1 2	
6.705E-01	1.020E+02	25	C045	2 2 0 1 2	
1.183E+00	1.800E+02	25	L035	1 2 2 1 2	
6.460E-01	9.829E+01	27.5	L035	1 2 2 1 2	
6.460E-01	9.829E+01	27.50	A043	1 2 1 1 2	
1.791E+00	2.725E+02	30	A043	1 2 1 1 2	
1.791E+00	2.725E+02	30	L035	1 2 2 1 2	
8.223E-01	1.251E+02	31.5	L035	1 2 2 1 2	
8.223E-01	1.251E+02	31.50	A043	1 2 1 1 2	
2.957E+00	4.499E+02	35	A043	1 2 1 1 2	
2.957E+00	4.499E+02	35	L035	1 2 2 1 2	
3.434E+00	5.224E+02	37	A043	1 2 1 1 2	
1.132E+00	1.722E+02	37	A043	1 2 1 1 2	
3.434E+00	5.224E+02	37	L035	1 2 2 1 2	
1.132E+00	1.722E+02	37	L035	1 2 2 1 2	
4.075E+00	6.201E+02	40	A043	1 2 1 1 2	
4.075E+00	6.201E+02	40	L035	1 2 2 1 2	
1.517E+00	2.308E+02	41.5	L035	1 2 2 1 2	
1.517E+00	2.308E+02	41.50	A043	1 2 1 1 2	
4.325E+00	6.580E+02	42.5	L035	1 2 2 1 2	
4.325E+00	6.580E+02	42.50	A043	1 2 1 1 2	
1.871E+00	2.847E+02	44	A043	1 2 1 1 2	
1.871E+00	2.847E+02	44	L035	1 2 2 1 2	
4.678E+00	7.118E+02	45	L035	1 2 2 1 2	
4.678E+00	7.118E+02	45.50	A043	1 2 1 1 2	
2.351E+00	3.577E+02	46.5	L035	1 2 2 1 2	
2.351E+00	3.577E+02	46.50	A043	1 2 1 1 2	
4.816E+00	7.328E+02	47	L035	1 2 2 1 2	
4.816E+00	7.328E+02	47.50	A043	1 2 1 1 2	
2.795E+00	4.253E+02	48.5	L035	1 2 2 1 2	
2.795E+00	4.253E+02	48.50	A043	1 2 1 1 2	
5.183E+00	7.886E+02	50	A043	1 2 1 1 2	
5.183E+00	7.886E+02	50	L035	1 2 2 1 2	
3.192E+00	4.856E+02	50.5	L035	1 2 2 1 2	
3.192E+00	4.856E+02	50.50	A043	1 2 1 1 2	
3.484E+00	5.301E+02	52.5	L035	1 2 2 1 2	
3.484E+00	5.301E+02	52.50	A043	1 2 1 1 2	
3.704E+00	5.635E+02	54.50	A043	1 2 1 1 2	
3.704E+00	5.635E+02	54.50	L035	1 2 2 1 2	
3.996E+00	6.080E+02	57	A043	1 2 1 1 2	

(continued)

1452. C₈H₈O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.996E+00	6.080E+02	57	L035	1 2 2 1 2	
4.337E+00	6.599E+02	60.5	L035	1 2 2 1 2	
4.337E+00	6.599E+02	60.50	A043	1 2 1 1 2	
4.884E+00	7.431E+02	68	A043	1 2 1 1 2	
4.884E+00	7.431E+02	68	L035	1 2 2 1 2	

1453. C₈H₈O₃*m*-Cresotic acid2-Hydroxy-*p*-tolylsaeure-(1)*m*-Kresotinsaeure

RN: 50-85-1

MP (°C): 177

MW: 152.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.638E-02	1.010E+01	100	F300	1 0 0 0 2	

1454. C₈H₈O₃*o*-Anisic acid

2-Methoxybenzoic acid

Salicylic acid methyl ether

Salicylsaeure-methylaether

o-Methoxybenzoic acid

RN: 579-75-9

MP (°C): 101

MW: 152.15

BP (°C): 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-02	1.567E+00	4.99	A405	2 0 1 1 2	
1.220E-02	1.856E+00	9.99	A405	2 0 1 1 2	
1.420E-02	2.161E+00	14.99	A405	2 0 1 1 2	
1.710E-02	2.602E+00	19.99	A405	2 0 1 1 2	
2.070E-02	3.150E+00	23.99	A405	2 0 1 1 2	
2.760E-02	4.200E+00	25	H007	0 0 0 0 0	
2.440E-02	3.712E+00	26.99	A405	2 0 1 1 2	
3.286E-02	5.000E+00	30	F300	1 0 0 0 0	
2.760E-02	4.199E+00	30.99	A405	2 0 1 1 2	
3.120E-02	4.747E+00	34.99	A405	2 0 1 1 2	
3.503E-02	5.330E+00	37	M360	1 2 1 1 2	
3.750E-02	5.706E+00	38.99	A405	2 0 1 1 2	
4.390E-02	6.679E+00	41.99	A405	2 0 1 1 2	
4.800E-02	7.303E+00	44.99	A405	2 0 1 1 2	
5.930E-02	9.023E+00	47.99	A405	2 0 1 1 2	
6.930E-02	1.054E+01	52.99	A405	2 0 1 1 2	
8.370E-02	1.274E+01	53.99	A405	2 0 1 1 2	
9.500E-02	1.445E+01	56.99	A405	2 0 1 1 2	
1.261E-01	1.919E+01	60.99	A405	2 0 1 1 2	
1.683E-01	2.561E+01	64.99	A405	2 0 1 1 2	

(continued)

1454. C₈H₈O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.326E-01	3.539E+01	68.99	A405	2 0 1 1 2	
2.630E-01	4.002E+01	69.99	A405	2 0 1 1 2	
3.467E-01	5.275E+01	72.99	A405	2 0 1 1 2	

1455. C₈H₈O₃

Mandelic acid

Amygdallic acid

α-Hydroxyphenylacetic acid

Uromaline

α-Hydroxy-benzeneacetic acid

RN: 90-64-2 MP (°C): 119.0

MW: 152.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.191E+00	1.812E+02	25	K040	1 0 2 1 2	<i>sic</i>
8.795E-03	1.338E+00	25	R049	0 0 0 0 0	
9.120E-01	1.388E+02	ns	R427	0 0 0 0 0	

1456. C₈H₈O₃3-Hydroxy-*p*-toluic acid3-Hydroxy-*p*-tolylsaeure-(I)

RN: 586-30-1 MP (°C):

MW: 152.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.859E-01	4.350E+01	100	F300	1 0 0 0 2	

1457. C₈H₈O₃

3-Methoxybenzoic acid

3-Methoxy-benzoesaeure

m-Anisic acid*m*-Methoxybenzoic acid

RN: 586-38-9 MP (°C): 110

MW: 152.15 BP (°C): 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.282E-02	1.950E+00	37	M360	1 2 1 1 2	
1.183E-03	1.800E-01	ns	B361	0 0 0 0 0	

1458. C₈H₈O₃

DL-Mandelic acid

DL-Mandelsaeure

RN: 611-72-3 MP (°C): 122

MW: 152.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.050E-01	1.377E+02	20	F300	1 0 0 0 2	
1.134E+00	1.725E+02	24	F300	1 0 0 0 2	

1459. C₈H₈O₃4-Hydroxy-*m*-toluic acid4-Hydroxy-*m*-tolylsaeure-(1)*o*-Cresotic acid2-Hydroxy-*m*-toluic acid2-Hydroxy-*m*-tolylsaeure-(1)

RN: 83-40-9 MP (°C): 165.5

MW: 152.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.624E-02	1.160E+01	100	F300	1 0 0 0 2	
3.411E-01	5.190E+01	100	F300	1 0 0 0 2	

1460. C₈H₈O₃

Phenoxyacetic acid

Glycolic acid phenyl ether

O-Phenylglycolic acid

RN: 122-59-8 MP (°C): 98

MW: 152.15 BP (°C): 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.887E-02	1.200E+01	10	F071	1 1 2 1 2	
8.084E-03	1.230E+00	10	F300	1 0 0 0 2	
7.887E-02	1.200E+01	10	H080	1 0 0 0 2	
7.887E-02	1.200E+01	10	M344	1 0 0 0 2	
1.100E-04	1.674E-02	25	L030	1 0 2 1 2	

1461. C₈H₈O₃*p*-Methoxybenzoic acid

4-Methoxybenzoic acid

p-Anisic acid

Anissaeure

RN: 100-09-4**MP (°C):** 184**MW:** 152.15**BP (°C):** 275

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-04	1.111E-01	2.99	A405	2 0 1 1 2	
9.400E-04	1.430E-01	4.99	A405	2 0 1 1 2	
1.070E-03	1.628E-01	10.99	A405	2 0 1 1 2	
1.270E-03	1.932E-01	14.99	A405	2 0 1 1 2	
1.775E-02	2.700E+00	19	F300	1 0 0 0 1	
1.330E-03	2.024E-01	19.99	A405	2 0 1 1 2	
1.680E-03	2.556E-01	24.99	A405	2 0 1 1 2	
2.020E-03	3.073E-01	28.99	A405	2 0 1 1 2	
2.300E-03	3.499E-01	33.99	A405	2 0 1 1 2	
3.483E-03	5.300E-01	37	B171	2 0 1 1 2	
1.380E-03	2.100E-01	37	M360	1 2 1 1 2	
3.110E-03	4.732E-01	39.99	A405	2 0 1 1 2	
3.870E-03	5.888E-01	43.99	A405	2 0 1 1 2	
5.130E-03	7.805E-01	50.99	A405	2 0 1 1 2	
6.110E-03	9.296E-01	55.99	A405	2 0 1 1 2	
8.170E-03	1.243E+00	59.99	A405	2 0 1 1 2	
9.000E-03	1.369E+00	64.99	A405	2 0 1 1 2	
1.080E-02	1.643E+00	65.99	A405	2 0 1 1 2	
1.100E-02	1.674E+00	66.99	A405	2 0 1 1 2	
1.460E-02	2.221E+00	71.99	A405	2 0 1 1 2	
1.778E-02	2.706E+00	ns	R427	0 0 0 0 0	

1462. C₈H₈O₃*p*-Cresotic acid6-Hydroxy-*m*-toluic acid6-Hydroxy-*m*-tolylsaeure-(1)**RN:** 89-56-5**MP (°C):** 151**MW:** 152.15**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.439E-01	2.190E+01	100	F300	1 0 0 0 2	

1463. C₈H₈O₄

Vanillic acid

Vanillinsaeure

RN: 121-34-6 **MP (°C):** 214
MW: 168.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.921E-03	1.500E+00	14	F300	1 0 0 0 1	
1.546E-01	2.600E+01	100	F300	1 0 0 0 2	

1464. C₈H₈O₄

Homogentisic acid

2,5-Dihydroxyphenylacetic acid

2,5-Dihydroxy-benzeneacetic acid

RN: 451-13-8 **MP (°C):** 151
MW: 168.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.732E+00	4.595E+02	25	D041	1 0 0 0 1	

1465. C₈H₈O₅

Methyl gallate

Gallussaeuremethyl ester

Methyl-3,4,5-trihydroxybenzoate

RN: 99-24-1 **MP (°C):** 201.5
MW: 184.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.323E-02	9.803E+00	19.99	L430	0 0 0 0 0	
5.696E-02	1.049E+01	24.99	L430	0 0 0 0 0	
6.757E-02	1.244E+01	29.99	L430	0 0 0 0 0	
9.549E-02	1.759E+01	34.99	L430	0 0 0 0 0	
1.340E-01	2.468E+01	39.99	L430	0 0 0 0 0	
1.704E-01	3.138E+01	44.99	L430	0 0 0 0 0	
2.542E-01	4.680E+01	49.99	L430	0 0 0 0 0	
4.328E-01	7.970E+01	54.99	L430	0 0 0 0 0	
5.879E-01	1.083E+02	59.99	L430	0 0 0 0 0	
7.775E-01	1.432E+02	64.99	L430	0 0 0 0 0	
1.054E+00	1.941E+02	69.99	L430	0 0 0 0 0	
1.624E-02	2.991E+00	-0	L430	0 0 0 0 0	
5.756E-02	1.060E+01	ns	F300	0 0 0 0 2	

1466. C₈H₉ClNO₅PS

Chlorthion

O,O-Dimethyl *O*-4-nitro-3-chlorophenyl thiophosphate

RN: 500-28-7 MP (°C): 21

MW: 297.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.344E-04	4.000E-02	20	M061	1 0 0 0 1	

1467. C₈H₉ClNO₅PS

Dicapthon

O-(2-Chloro-4-nitrophenyl) *O,O*-dimethyl phosphorothioate

Dicaptan

Isochlorthion

RN: 2463-84-5 MP (°C):

MW: 297.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.233E-05	1.260E-02	10	B324	0 0 0 0 0	
4.233E-05	1.260E-02	10	B324	0 0 0 0 0	
4.939E-05	1.470E-02	20	B300	2 1 1 1 2	
4.939E-05	1.470E-02	20	B324	0 0 0 0 0	
4.939E-05	1.470E-02	20	B324	0 0 0 0 0	
2.100E-05	6.250E-03	20	C053	0 0 0 0 0	
1.485E-04	4.420E-02	30	B324	0 0 0 0 0	
1.485E-04	4.420E-02	30	B324	0 0 0 0 0	
2.100E-05	6.250E-03	ns	F071	0 1 2 1 2	
1.176E-04	3.500E-02	ns	M061	0 0 0 0 1	
2.620E-05	7.800E-03	rt	F040	1 2 2 2 1	

1468. C₈H₉ClO

2,5-Dimethyl-4-chloro-phenol

4-Chloro-2,5-xylenol

4-Chloro-2,5-dimethylphenol

RN: 1124-06-7 MP (°C): 114–116

MW: 156.61 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	8.927E+00	25	B316	0 0 0 0 0	

1469. C₈H₉ClO

2,6-Dimethyl-4-chloro-phenol

4-Chloro-2,6-xylenol

RN: 1123-63-3 MP (°C):

MW: 156.61 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-03	5.168E-01	25	B316	0 0 0 0 0	

1470. C₈H₉ClO

Chloroxylenol

3,5-Dimethyl-4-chloro-phenol-

RN: 88-04-0 **MP (°C):** 115.5
MW: 156.61 **BP (°C):** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E-03	2.500E-01	20	M018	1 2 2 1 0	
1.979E-03	3.099E-01	20	M093	1 0 0 1 1	
2.200E-02	3.445E+00	25	B316	0 0 0 0 0	<i>sic</i>
1.915E-03	2.999E-01	25	R041	0 0 0 0 0	
1.585E-03	2.482E-01	ns	R427	0 0 0 0 0	

1471. C₈H₉FN₂O₃

2,4(1H,3H)-Pyrimidinedione, 5-fluoro-3-(1-oxobutyl)-

RN: 94452-21-8 **MP (°C):**
MW: 200.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-02	1.061E+01	22	B416	2 2 1 2 1	

1472. C₈H₉FN₂O₃

Ftorafur

THFFU

1-(2-Tetrahydrofuryl)-5-fluorouracil

RN: 37076-68-9 **MP (°C):** 167
MW: 200.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-01	2.802E+01	37	N017	0 0 0 0 0	

1473. C₈H₉FN₂O₄

1-Propionyloxymethyl-5-fluorouracil

1-Propionyloxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

RN: 66542-36-7 **MP (°C):** 100-102
MW: 216.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E-01	3.360E+01	22	B321	0 0 0 0 0	pH 4.0

1474. C₈H₉FN₂O₄

1-Isopropoxyarbonyl-5-fluorouracil

1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, 1-methylethyl ester

RN: 109232-73-7 MP (°C): 180

MW: 216.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.174E-02	4.700E+00	22	B332	1 1 0 0 1	pH 4.0

1475. C₈H₉N

Indoline

2,3-Dihydro-1H-indole

2,3-Dihydroindole

RN: 496-15-1 MP (°C): <25

MW: 119.17 BP (°C): 220.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.934E-02	3.497E+00	20.3	L339	2 0 2 2 2	
9.063E-02	1.080E+01	25	P051	2 1 1 2 2	
9.063E-02	1.080E+01	25.00	P007	2 1 2 2 1	
3.651E-02	4.350E+00	40.0	L339	2 0 2 2 2	
4.586E-02	5.465E+00	59.4	L339	2 0 2 2 2	
5.738E-02	6.838E+00	79.0	L339	2 0 2 2 2	
8.142E-02	9.703E+00	100.0	L339	2 0 2 2 2	

1476. C₈H₉NO*p*-Aminoacetophenone

4'-Aminoacetophenone

RN: 99-92-3 MP (°C): 106

MW: 135.17 BP (°C): 294

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.480E-02	3.352E+00	37.5	G002	1 1 1 1 2	

1477. C₈H₉NO

Acetanilide

Acetanilid

RN: 103-84-4 MP (°C): 114

MW: 135.17 BP (°C): 304

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.652E-02	3.585E+00	0	L029	2 2 2 2 2	
3.534E-02	4.777E+00	10	M043	1 0 0 0 1	
3.251E-02	4.395E+00	10.1	L029	2 2 2 2 2	
2.970E-02	4.014E+00	14	O016	1 0 0 0 2	
3.688E-02	4.985E+00	15	L038	1 0 1 0 2	

(continued)

1477. C₈H₉NO (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.710E-02	5.015E+00	20	B101	0 0 0 0 0	
3.666E-02	4.955E+00	20	K078	1 0 2 1 2	
4.129E-02	5.581E+00	20	L029	2 2 2 2 2	
3.827E-02	5.173E+00	20	M043	1 0 0 0 1	
3.330E-02	4.501E+00	20	O019	1 0 0 1 2	
3.884E-02	5.250E+00	20	W026	1 0 1 1 1	average of 2
4.142E-02	5.598E+00	25	B101	0 0 0 0 0	
4.450E-02	6.015E+00	25	B434	0 0 0 0 0	
4.786E-02	6.468E+00	25	B434	0 0 0 0 0	
4.160E-02	5.623E+00	25	D044	0 0 0 0 0	
4.143E-02	5.600E+00	25	F300	1 0 0 0 1	
4.697E-02	6.349E+00	25	L029	2 2 2 2 2	
4.486E-02	6.063E+00	25	M094	1 0 0 1 1	
3.699E-02	5.000E+00	25	P016	1 0 0 1 0	
4.887E-02	6.606E+00	30	B101	0 0 0 0 0	
5.262E-02	7.113E+00	30	B434	0 0 0 0 0	
5.240E-02	7.083E+00	30	B434	0 0 0 0 0	
5.351E-02	7.232E+00	30	L029	2 2 2 2 2	
4.632E-02	6.261E+00	30	M043	1 0 0 0 1	
5.253E-02	7.100E+00	30	W026	1 0 1 1 1	average of 2
5.792E-02	7.828E+00	32.6	L038	1 0 1 0 2	
5.930E-02	8.015E+00	35	B101	0 0 0 0 0	
5.799E-02	7.838E+00	35	B434	0 0 0 0 0	
5.760E-02	7.786E+00	35	B434	0 0 0 0 0	
6.787E-02	9.174E+00	40	B434	0 0 0 0 0	
6.730E-02	9.097E+00	40	B434	0 0 0 0 0	
7.134E-02	9.643E+00	40	L029	2 2 2 2 2	
6.381E-02	8.625E+00	40	M043	1 0 0 0 1	
9.682E-02	1.309E+01	50	L029	2 2 2 2 2	
1.349E-01	1.823E+01	60	L029	2 2 2 2 2	
1.522E-01	2.057E+01	60	M043	1 0 0 0 1	
1.928E-01	2.606E+01	70	L029	2 2 2 2 2	
3.321E-01	4.489E+01	80	M043	1 0 0 0 1	
4.047E-02	5.470E+00	rt	D021	0 0 1 1 1	

1478. C₈H₉NO*m*-Aminoacetophenone

3'-Aminoacetophenone

RN: 99-03-6

MP (°C): 97

MW: 135.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.220E-02	7.056E+00	37.5	G002	1 1 1 1 2	pH 6.8

1479. C₈H₉NO₂

Acetaminophen

4-Acetamidophenol

4-Amino-phenol-*N*-acetat*p*-Acetaminophen*p*-Hydroxyacetanilide**RN:** 103-90-2**MP (°C):** 167**MW:** 151.17**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.307E-02	1.105E+01	15	M352	1 1 1 1 2	
5.462E-01	8.257E+01	16.9	Y412	0 0 0 0 0	
6.014E-01	9.091E+01	21.5	Y412	0 0 0 0 0	
1.323E-01	2.000E+01	25	B010	1 1 1 1 0	
1.016E-01	1.536E+01	25	B434	0 0 0 0 0	
9.500E-02	1.436E+01	25	C032	2 2 1 2 0	EFG
7.710E-02	1.165E+01	25	D044	0 0 0 0 0	
9.133E-02	1.381E+01	25	D078	1 2 1 1 2	
5.185E-02	7.838E+00	25	F415	0 0 0 0 0	Average
1.000E-01	1.512E+01	25	K041	1 0 0 0 0	
9.851E-02	1.489E+01	25	M352	1 1 1 1 2	
9.923E-02	1.500E+01	25	P016	1 0 0 1 1	
7.277E-02	1.100E+01	25	P312	0 0 0 0 0	
9.326E-02	1.410E+01	25	W019	1 0 1 1 2	
3.538E-01	5.348E+01	25	Y410	0 0 0 0 0	
9.140E-02	1.382E+01	25	Z408	0 0 0 0 0	
6.556E-01	9.910E+01	26.3	Y412	0 0 0 0 0	
1.241E-01	1.876E+01	30	B434	0 0 0 0 0	
1.240E-01	1.874E+01	30	B434	0 0 0 0 0	
1.120E-01	1.693E+01	30	L069	1 0 1 1 0	EFG
7.088E-01	1.071E+02	31.5	Y412	0 0 0 0 0	
1.684E-01	2.545E+01	35	B434	0 0 0 0 0	
1.684E-01	2.546E+01	35	B434	0 0 0 0 0	
7.610E-01	1.150E+02	35.3	Y412	0 0 0 0 0	
1.323E-01	2.000E+01	37	F076	2 0 2 2 0	
1.442E-01	2.180E+01	37	K086	1 0 0 0 2	
8.124E-01	1.228E+02	37	Y412	0 0 0 0 0	
1.349E-01	2.039E+01	39.3	G302	2 0 2 2 0	EFG
2.234E-01	3.377E+01	40	B434	0 0 0 0 0	
2.238E-01	3.384E+01	40	B434	0 0 0 0 0	
1.440E-01	2.177E+01	40	M352	1 1 1 1 2	
1.800E-01	2.720E+01	50	M352	1 1 1 1 2	
1.019E-01	1.540E+01	c	B434	0 0 0 0 0	
6.615E-04	1.000E-01	ns	K444	0 0 0 0 0	
8.004E-02	1.210E+01	rt	R431	0 0 0 0 0	Average

1480. C₈H₉NO₂

Benzyl carbamate

O-Benzyl carbamate

Benzoyloxycarbonyl amine

RN: 621-84-1 MP (°C): 87

MW: 151.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-01	6.802E+01	37	H006	1 2 2 1 1	
4.467E-01	6.752E+01	ns	R427	0 0 0 0 0	

1481. C₈H₉NO₂

DL-2-Phenylglycine

2-Amino-phenyl-essigsaeure

2-Aminophenylacetic acid

RN: 2835-06-5 MP (°C): 255

MW: 151.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.608E-01	1.150E+02	100	F300	1 0 0 0 2	

1482. C₈H₉NO₂

N-Methylanthranilic acid

N-Methyl-anthranilsaure

RN: 119-68-6 MP (°C): 171

MW: 151.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.323E-03	2.000E-01	20	F300	1 0 0 0 2	
2.646E-03	4.000E-01	100	F300	1 0 0 0 2	

1483. C₈H₉NO₂

D-Phenylglycine

D-2-Phenylglycine

D-(–)-α-Aminophenylacetic acid

Benzeneacetic acid, α-amino-

RN: 875-74-1 MP (°C): 302 C

MW: 151.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.034E-02	4.586E+00	25	R419	0 0 0 0 0	

1484. C₈H₉NO₂Methyl-*p*-aminobenzoateMethyl *p*-aminobenzoate

4-Aminobenzoic acid methyl ester

RN: 619-45-4 **MP (°C):****MW:** 151.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.884E-03	8.894E-01	15	M352	1 1 1 1 2	
9.542E-03	1.442E+00	25	M352	1 1 1 1 2	
1.070E-02	1.618E+00	25	P303	0 0 0 0 0	
1.397E-02	2.112E+00	33	P303	0 0 0 0 0	
2.530E-02	3.825E+00	37	F006	1 1 2 2 2	
1.646E-02	2.488E+00	40	M352	1 1 1 1 2	
1.839E-02	2.780E+00	40	P303	0 0 0 0 0	
7.940E-03	1.200E+00	ns	M066	0 0 0 0 2	
7.940E-03	1.200E+00	rt	B016	0 0 1 1 2	pH 7.4

1485. C₈H₉NO₂S₂

2-(2-Thienyl)-L-thiazolidine-4-carboxylic acid

4-Thiazolidinecarboxylic acid, 2-(2-thienyl)-

RN: 32451-19-7 **MP (°C):****MW:** 215.29 **BP (°C):** 454.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	1.055E+00	21	B414	1 0 0 1 1	fast decomposition

1486. C₈H₉NO₃D-(*p*-hydroxy)phenylglycine**RN:** **MP (°C):****MW:** 167.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-01	1.937E+01	25	R419	0 0 0 0 0	

1487. C₈H₉NO₃S*p*-Acetylbenzenesulfonamide

4-Acetylbenzenesulfonamide

RN: 1565-17-9 **MP (°C):****MW:** 199.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	4.582E-01	15	K024	1 2 1 1 2	

1488. C₈H₉NO₄

Biliverdic acid

Biliverdinsaeure

RN: 487-65-0 **MP (°C):**
MW: 183.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.129E-01	3.900E+01	20	F300	1 0 0 0 1	

1489. C₈H₉N₃O₃

Orotic acid allylamide

4-Pyrimidinecarboxamide, 1,2,3,6-tetrahydro-2,6-dioxo-*N*-2-propenyl-

RN: 292870-71-4 **MP (°C):** 259–262
MW: 195.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E-01	3.474E+01	−4	N018	0 0 0 0 0	
3.000E-01	5.855E+01	16	N018	0 0 0 0 0	
3.710E-01	7.241E+01	25	N018	0 0 0 0 0	

1490. C₈H₉N₅

7-Dimethylaminopteridine

7-Pteridinamine, *N,N*-dimethyl-

RN: 204443-26-5 **MP (°C):**
MW: 175.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.154E-01	1.429E+02	20	A083	1 2 0 0 0	
1.903E+00	3.333E+02	100	A083	1 2 0 0 0	

1491. C₈H₉N₅

2-Dimethylaminopteridine

2-Pteridinamine, *N,N*-dimethyl-

RN: 41047-52-3 **MP (°C):**
MW: 175.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.631E+00	2.857E+02	22.5	A085	1 2 0 0 0	

1492. C₈H₉N₅

4-Dimethylaminopteridine

4-Pteridinamine, *N,N*-dimethyl-

RN: 14131-04-5 MP (°C): 165

MW: 175.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.357E-02	1.639E+01	20	A019	2 2 1 1 0	
1.392E-01	2.439E+01	100	A019	1 2 1 1 0	

1493. C₈H₉O₃PS

2-Methoxy-4H-benzo-1,3,2-dioxaphosphorin-2-thione

Dioxabenzofos

Salithion

Fenfosphorin

Dioxabenzophos

RN: 3811-49-2 MP (°C): 55.5

MW: 216.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.683E-04	5.800E-02	30	M161	1 0 0 0 1	

1494. C₈H₁₀

Ethylbenzene

Phenylethane

Ethylenzene

Ethylbenzol

EB

RN: 100-41-4 MP (°C): -95

MW: 106.17 BP (°C): 136.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.856E-03	1.970E-01	0	P003	2 2 2 2 2	
1.846E-03	1.960E-01	4.50	B086	2 1 2 2 2	
1.808E-03	1.920E-01	6.30	B086	2 1 2 2 2	
1.677E-03	1.781E-01	7.09	F418	0 0 0 0 0	
1.752E-03	1.860E-01	7.10	B086	2 1 2 2 2	
1.761E-03	1.870E-01	9	B086	2 1 2 2 2	
1.910E-03	2.028E-01	10	B149	2 1 1 2 2	
1.850E-03	1.964E-01	10	O312	2 2 0 2 2	
1.705E-03	1.810E-01	11.80	B086	2 1 2 2 2	
1.723E-03	1.830E-01	12.10	B086	2 1 2 2 2	
1.812E-03	1.924E-01	14	O312	2 2 0 2 2	
1.300E-03	1.380E-01	15	F001	1 0 1 2 1	
1.300E-03	1.380E-01	15	S006	1 0 0 0 1	
1.658E-03	1.760E-01	15	S203	1 1 2 1 2	
1.695E-03	1.800E-01	15.10	B086	2 1 2 2 2	

(continued)

1494. C₈H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.639E-03	1.740E-01	16.93	F418	0 0 0 0 0	
1.776E-03	1.886E-01	17	O312	2 2 0 2 2	
1.733E-03	1.840E-01	17.90	B086	2 1 2 2 2	
2.901E-03	3.080E-01	18	F185	1 0 0 0 2	
2.788E-03	2.960E-01	18	F185	1 0 0 0 2	
1.725E-03	1.831E-01	18	O312	2 2 0 2 2	
3.080E-03	3.270E-01	19	F185	1 0 0 0 2	
1.676E-03	1.779E-01	19	O312	2 2 0 2 2	
2.000E-03	2.123E-01	20	B149	2 1 1 2 2	
1.695E-03	1.800E-01	20	B356	0 0 0 0 0	
1.770E-03	1.879E-01	20	O312	2 2 0 2 2	
1.695E-03	1.800E-01	20.10	B086	2 1 2 2 1	
1.724E-03	1.830E-01	21	O312	2 2 0 2 2	
3.297E-03	3.500E-01	22	F185	1 0 0 0 2	
1.713E-03	1.819E-01	22	O312	2 2 0 2 2	
3.391E-03	3.600E-01	23	F185	1 0 0 0 2	
1.751E-03	1.859E-01	23.5	O312	2 2 0 2 2	
3.655E-03	3.880E-01	24	F185	1 0 0 0 2	
1.582E-03	1.680E-01	25	A002	1 2 1 1 2	
1.883E-03	2.000E-01	25	A094	1 0 0 0 0	
1.959E-03	2.080E-01	25	B003	2 2 2 2 2	
1.432E-03	1.520E-01	25	B060	2 0 1 1 1	
2.000E-03	2.123E-01	25	B153	2 1 1 1 2	
1.640E-03	1.741E-01	25	K001	1 0 2 1 2	
1.319E-03	1.400E-01	25	K072	1 0 1 1 1	
1.760E-03	1.869E-01	25	M342	1 0 1 1 2	
1.811E-03	1.923E-01	25	O312	2 2 0 2 2	
1.667E-03	1.770E-01	25	P003	2 2 2 2 2	
1.234E-03	1.310E-01	25	P051	2 1 1 2 2	
1.705E-03	1.810E-01	25	S203	1 1 2 1 2	
1.518E-03	1.612E-01	25	S358	2 1 2 2 2	
1.370E-03	1.455E-01	25	S359	2 1 2 2 2	
1.760E-03	1.869E-01	25	W300	2 2 2 2 2	
1.959E-03	2.080E-01	25.0	G035	1 0 0 0 2	
1.753E-03	1.861E-01	25.8	O312	2 2 0 2 2	
1.705E-03	1.810E-01	26.74	F418	0 0 0 0 0	
4.653E-03	4.940E-01	27	F185	1 0 0 0 2	
1.677E-03	1.780E-01	28	B348	2 1 2 2 2	
1.747E-03	1.855E-01	28	O312	2 2 0 2 2	
5.604E-03	5.950E-01	29	F185	1 0 0 0 2	
1.600E-03	1.698E-01	29.99	C350	0 0 0 0 0	
1.391E-03	1.477E-01	30	M311	1 1 2 2 2	
1.777E-03	1.887E-01	30	O312	2 2 0 2 2	
6.103E-03	6.480E-01	31	F185	1 0 0 0 2	
6.395E-03	6.790E-01	32	F185	1 0 0 0 2	
7.017E-03	7.450E-01	34	F185	1 0 0 0 2	
7.319E-03	7.770E-01	35	F185	1 0 0 0 2	
1.818E-03	1.930E-01	35	O312	2 2 0 2 2	
1.827E-03	1.940E-01	35	S203	1 1 2 1 2	

(continued)

1494. C₈H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.865E-03	8.350E-01	36	F185	1 0 0 0 2	
1.805E-03	1.917E-01	36.55	F418	0 0 0 0 0	
8.637E-03	9.170E-01	38	F185	1 0 0 0 2	
1.622E-03	1.722E-01	39.99	C350	0 0 0 0 0	
1.928E-03	2.047E-01	40	O312	2 2 0 2 2	
9.466E-03	1.005E+00	41	F185	1 0 0 0 2	
1.991E-03	2.114E-01	45	O312	2 2 0 2 2	
2.025E-03	2.150E-01	45	S203	1 1 2 1 2	
1.994E-03	2.117E-01	46.49	F418	0 0 0 0 0	
1.154E-02	1.225E+00	47	F185	1 0 0 0 2	
1.224E-02	1.300E+00	49	F185	1 0 0 0 2	
1.861E-03	1.976E-01	49.99	C350	0 0 0 0 0	
2.216E-03	2.353E-01	56.73	F418	0 0 0 0 0	
2.261E-03	2.400E-01	59.99	C350	0 0 0 0 0	
2.560E-03	2.718E-01	66.64	F418	0 0 0 0 0	
2.738E-03	2.907E-01	69.99	C350	0 0 0 0 0	
3.327E-03	3.532E-01	79.99	C350	0 0 0 0 0	
3.860E-03	4.098E-01	89.99	C350	0 0 0 0 0	
4.742E-03	5.035E-01	99.99	C350	0 0 0 0 0	
4.829E-03	5.127E-01	115.0	G035	1 0 0 0 2	
1.120E-02	1.189E+00	140.5	G035	1 0 0 0 2	
3.332E-02	3.537E+00	170.5	G035	1 0 0 0 2	
6.185E-02	6.567E+00	210.0	G035	1 0 0 0 2	
1.052E-01	1.116E+01	233.5	G035	1 0 0 0 2	
1.432E-03	1.520E-01	ns	H123	0 0 0 0 0	
6.300E-02	6.689E+00	ns	H307	0 0 0 0 0	
1.432E-03	1.520E-01	ns	M344	0 0 0 0 2	

1495. C₈H₁₀*m*-Xylene

1,3-Xylene

RN: 108-38-3

MP (°C): -47.4

MW: 106.17

BP (°C): 139.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.846E-03	1.960E-01	0	P003	2 2 2 2 2	
1.463E-03	1.554E-01	20	M337	2 1 2 2 2	
1.629E-03	1.730E-01	25	A001	1 2 2 2 2	
1.846E-03	1.960E-01	25	B003	2 2 2 2 2	
1.262E-03	1.340E-01	25	K119	1 0 0 0 2	
1.510E-03	1.603E-01	25	M342	1 0 1 1 2	
1.526E-03	1.620E-01	25	P003	2 2 2 2 2	
1.262E-03	1.340E-01	25	P051	2 1 1 2 2	
1.375E-03	1.460E-01	25	S005	2 2 2 2 2	
1.375E-03	1.460E-01	25	S191	1 2 2 2 2	
1.375E-03	1.460E-01	25	S358	2 1 2 2 2	
1.330E-03	1.412E-01	25	S359	2 1 2 2 2	

(continued)

1495. C₈H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.510E-03	1.603E-01	25	W300	2 2 2 2 2	
1.262E-03	1.340E-01	25.00	P007	2 1 2 2 2	
1.940E-03	2.059E-01	25.04	V013	2 2 2 2 2	
3.277E-03	3.479E-01	67.7	P005	1 1 2 1 2	
6.257E-03	6.643E-01	107.3	P005	1 1 2 1 2	
9.707E-03	1.031E+00	124.2	P005	1 1 2 1 2	
2.363E-02	2.509E+00	164.2	P005	1 1 2 1 2	
4.327E-02	4.594E+00	186.4	P005	1 1 2 1 2	
4.293E-02	4.557E+00	189.9	P005	1 1 2 1 2	
2.675E-01	2.840E+01	266.6	P005	1 1 2 1 2	
2.698E-01	2.865E+01	270.6	P005	1 1 2 1 2	

1496. C₈H₁₀*o*-Xylene

1,2-Dimethylbenzene

1,2-Xylene

RN: 95-47-6 **MP (°C):** -25
MW: 106.17 **BP (°C):** 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.337E-03	1.420E-01	0	P003	2 2 2 2 2	
2.000E-03	2.123E-01	10	B149	2 1 1 2 2	
2.260E-03	2.399E-01	20	B149	2 1 1 2 2	
1.605E-03	1.704E-01	20	M337	2 1 2 2 2	
1.921E-03	2.040E-01	25	A001	1 2 2 2 2	
1.648E-03	1.750E-01	25	B060	2 0 1 1 1	
1.573E-03	1.670E-01	25	K119	1 0 0 0 2	
1.648E-03	1.750E-01	25	M001	2 1 2 2 2	
1.648E-03	1.750E-01	25	M002	2 1 2 2 2	
1.648E-03	1.750E-01	25	M040	1 0 0 1 2	
1.648E-03	1.750E-01	25	M130	1 0 0 0 2	
2.080E-03	2.208E-01	25	M342	1 0 1 1 2	
2.006E-03	2.130E-01	25	P003	2 2 2 2 2	
1.573E-03	1.670E-01	25	P051	2 1 1 2 2	
1.606E-03	1.705E-01	25	S005	2 2 2 2 2	
1.606E-03	1.705E-01	25	S191	1 2 2 2 2	
1.606E-03	1.705E-01	25	S358	2 1 2 2 2	
1.680E-03	1.784E-01	25	S359	2 1 2 2 2	
2.080E-03	2.208E-01	25	W300	2 2 2 2 2	
1.573E-03	1.670E-01	25.00	P007	2 1 2 2 2	
1.272E-03	1.350E-01	ns	B150	0 0 2 2 2	
1.648E-03	1.750E-01	ns	M344	0 0 0 0 2	

1497. C₈H₁₀*p*-Xylene

1,4-Dimethylbenzene

1,4-Xylene

RN: 106-42-3 **MP (°C):** 13
MW: 106.17 **BP (°C):** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.545E-03	1.640E-01	0	P003	2 2 2 2 2	
1.780E-03	1.890E-01	10	B149	2 1 1 2 2	
1.800E-03	1.911E-01	20	B149	2 1 1 2 2	
1.552E-03	1.648E-01	20	M337	2 1 2 2 2	
1.884E-03	2.000E-01	25	A001	1 2 2 2 2	
1.865E-03	1.980E-01	25	B003	2 2 2 2 2	
1.224E-03	1.300E-01	25	K072	1 0 1 1 1	
1.479E-03	1.570E-01	25	K119	1 0 0 0 2	
1.789E-03	1.900E-01	25	L319	1 0 2 1 1	
1.224E-03	1.300E-01	25	M087	1 1 2 1 1	
2.020E-03	2.145E-01	25	M342	1 0 1 1 2	
1.743E-03	1.850E-01	25	P003	2 2 2 2 2	
1.479E-03	1.570E-01	25	P051	2 1 1 2 2	
1.469E-03	1.560E-01	25	S005	2 2 2 2 2	
1.469E-03	1.560E-01	25	S191	1 2 2 2 2	
1.469E-03	1.560E-01	25	S358	2 1 2 2 2	
1.510E-03	1.603E-01	25	S359	2 1 2 2 2	
2.020E-03	2.145E-01	25	W300	2 2 2 2 2	
1.479E-03	1.570E-01	25.00	P007	2 1 2 2 2	
1.589E-03	1.687E-01	29.99	C350	0 0 0 0 0	
1.766E-03	1.875E-01	39.99	C350	0 0 0 0 0	
2.410E-03	2.559E-01	43.0	P005	1 1 2 1 2	
1.911E-03	2.029E-01	49.99	C350	0 0 0 0 0	
2.832E-03	3.007E-01	56.4	P005	1 1 2 1 2	
2.244E-03	2.382E-01	59.99	C350	0 0 0 0 0	
3.199E-03	3.396E-01	65.0	P005	1 1 2 1 2	
2.683E-03	2.848E-01	69.99	C350	0 0 0 0 0	
3.643E-03	3.868E-01	75.3	P005	1 1 2 1 2	
3.171E-03	3.367E-01	79.99	C350	0 0 0 0 0	
4.326E-03	4.593E-01	87.2	P005	1 1 2 1 2	
3.721E-03	3.950E-01	89.99	C350	0 0 0 0 0	
4.853E-03	5.152E-01	99.99	C350	0 0 0 0 0	
2.363E-02	2.509E+00	162.5	P005	1 1 2 1 2	
4.251E-02	4.513E+00	188.1	P005	1 1 2 1 2	
1.614E-01	1.713E+01	243.2	P005	1 1 2 1 2	
4.053E-01	4.303E+01	282.5	P005	1 1 2 1 2	
4.011E-01	4.258E+01	294.9	P005	1 1 2 1 2	
1.743E-03	1.850E-01	ns	H123	0 0 0 0 0	

1498. C₈H₁₀

Xylene

Dimethylbenzene

Xylol

RN: 1330-20-7**MP (°C):****MW:** 106.17**BP (°C):** 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.469E-03	8.992E-01	20	C121	1 0 0 0 0	unit assumed, <i>sic</i>
1.000E-03	1.062E-01	25	H332	2 2 2 2 0	
<9.41E-03	<9.99E-01	25.50	O005	2 0 2 2 0	
9.419E-03	1.000E+00	150	J023	1 1 2 2 0	
3.297E-02	3.500E+00	200	J023	1 1 2 2 1	
1.036E-01	1.100E+01	250	J023	1 1 2 2 1	

1499. C₈H₁₀NO₅PS

Methyl parathion

Parathion-methyl

Methylparathion

RN: 298-00-0**MP (°C):** 36**MW:** 263.21**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.282E-05	2.180E-02	10	B324	0 0 0 0 0	
8.283E-05	2.180E-02	10	B324	0 0 0 0 0	
1.432E-04	3.770E-02	19.50	B169	2 2 1 1 2	
1.444E-04	3.801E-02	20	B324	0 0 0 0 0	
1.444E-04	3.800E-02	20	B324	0 0 0 0 0	
9.498E-05	2.500E-02	20	M040	1 0 0 1 1	
2.090E-04	5.500E-02	25	M061	1 0 0 0 1	
2.185E-04	5.750E-02	25	M161	1 0 0 0 0	
2.089E-04	5.500E-02	25	Z409	0 0 0 0 0	EFG
2.223E-04	5.851E-02	30	B324	0 0 0 0 0	
2.222E-04	5.850E-02	30	B324	0 0 0 0 0	
1.900E-04	5.000E-02	ns	C117	0 0 0 0 0	
1.445E-04	3.805E-02	ns	R427	0 0 0 0 0	
1.432E-04	3.770E-02	ns	V414	0 0 0 0 0	

1500. C₈H₁₀N₂O*p*-Phenylenediaminemono-*N*-acetate*p*-Phenylenediamin-mono-*N*-acetat**RN:** 589-29-7**MP (°C):****MW:** 150.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-01	6.200E+01	57	F300	1 0 0 0 1	

1501. C₈H₁₀N₂O*m*-Aminoacetanilide

3-Aminoacetanilide

RN: 102-28-3**MP (°C):****MW:** 150.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.526E-01	8.299E+01	48.7	S115	1 2 1 1 2	
1.021E+00	1.534E+02	82.9	S115	1 2 1 1 2	

1502. C₈H₁₀N₂O*o*-Aminoacetanilide

2-Aminoacetanilide

RN: 34801-09-7**MP (°C):****MW:** 150.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.189E-01	3.288E+01	7.2	S115	1 2 1 1 2	
7.161E-01	1.075E+02	22.0	S115	1 2 1 1 2	
1.215E+00	1.825E+02	33.5	S115	1 2 1 1 2	
1.612E+00	2.421E+02	42.1	S115	1 2 1 1 2	
1.958E+00	2.940E+02	50.4	S115	1 2 1 1 2	
2.270E+00	3.409E+02	59.1	S115	1 2 1 1 2	
2.601E+00	3.906E+02	69.9	S115	1 2 1 1 2	
2.781E+00	4.177E+02	78.2	S115	1 2 1 1 2	
2.943E+00	4.420E+02	88.1	S115	1 2 1 1 2	
3.075E+00	4.618E+02	99.0	S115	1 2 1 1 2	
3.213E+00	4.825E+02	115.4	S115	1 2 1 1 2	

1503. C₈H₁₀N₂O

1-(2-Tolyl)urea

o-Tolylurea**RN:** 614-77-7**MP (°C):****MW:** 150.18**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-02	2.504E+00	45	W044	1 0 1 0 2	

1504. C₈H₁₀N₂O

1-Methyl-3-phenylurea

Desfenuron

N-Phenyl-N'-methylurea

Desphenuron

N-Methyl-N'-phenylurea

IPO 4328

RN: 1007-36-9 MP (°C):

MW: 150.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.927E+00	7.400E+02	45	W044	1 0 1 0 2	

1505. C₈H₁₀N₂O

1-(4-Tolyl)urea

p-Tolylurea

RN: 622-51-5 MP (°C):

MW: 150.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.044E-02	3.070E+00	45	W044	1 0 1 0 2	

1506. C₈H₁₀N₂O*p*-Aminoacetanilide

4-Aminoacetanilide

RN: 122-80-5 MP (°C): 164.5

MW: 150.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.061E-01	1.593E+01	25	D044	0 0 0 0 0	
4.064E-01	6.103E+01	56.8	S115	1 2 1 1 2	
1.046E+00	1.570E+02	86.3	S115	1 2 1 1 2	
1.441E+00	2.165E+02	92.1	S115	1 2 1 1 2	
1.699E+00	2.552E+02	93.7	S115	1 2 1 1 2	
1.996E+00	2.998E+02	96.5	S115	1 2 1 1 2	
2.193E+00	3.293E+02	98.6	S115	1 2 1 1 2	

1507. C₈H₁₀N₂O

Methylbenzylnitrosamine

N-Nitroso(methyl)benzylamine

N-Nitroso-*N*-methylbenzylamine

N-Nitroso(benzyl)methylamine

N-Nitroso-*N*-methylbenzenemethanamine

RN: 937-40-6 MP (°C):

MW: 150.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	4.505E+00	24	D083	2 0 0 1	

1508. C₈H₁₀N₂O

Benzylurea

Benzyl-harnstoff

RN: 538-32-9 MP (°C): 147

MW: 150.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-01	1.700E+01	45	F300	1 0 0 2	
1.139E-01	1.710E+01	45	W044	1 0 1 0 2	

1509. C₈H₁₀N₂O₃

5-Methyl-5-allylbarbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-(2-propenyl)

5-Methyl-5-allylbarbiturate

RN: 143585-01-7 MP (°C):

MW: 182.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.920E-02	1.261E+01	25	P350	0 0 0 0 0	intrinsic

1510. C₈H₁₀N₂O₃

5,5-Tetramethylenebarbituric acid

7,9-Diazaspiro[4.5]decane-6,8,10-trione

Spirocyclopentabarbituric acid

Cyclopentane-spirobarbiturate

RN: 56209-30-4 MP (°C):

MW: 182.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.476E-03	8.154E-01	25	P350	0 0 0 0 0	intrinsic

1511. C₈H₁₀N₂O₃S*N*1-Acetylsulfanilamide

Sulfacetamide

Acetyl sulfacetamide

RN: 144-80-9**MP (°C):** 183**MW:** 214.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.881E-02	1.260E+01	20	F073	1 2 2 2 2	
3.871E-02	8.293E+00	25	M440	0 0 0 0 0	
5.834E-03	1.250E+00	37	B046	1 0 2 2 2	pH 4.5
5.834E-02	1.250E+01	37	B046	1 0 2 2 2	pH 5
6.908E-02	1.480E+01	37	D084	1 0 1 0 2	
5.601E-02	1.200E+01	37	K086	1 0 0 0 2	
5.134E-02	1.100E+01	37	L091	1 0 0 0 2	pH 5.5
2.327E-02	4.985E+00	ns	L044	0 0 0 0 2	
3.090E-02	6.621E+00	ns	R427	0 0 0 0 0	

1512. C₈H₁₀N₂O₃S*N*4-Acetylsulfanilamide*N*4-Acetyl sulphanilamide**RN:** 121-61-9**MP (°C):** 216**MW:** 214.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.474E-02	5.300E+00	37	L091	1 0 0 0 2	pH 5.5
2.479E-02	5.312E+00	37.50	M142	1 0 0 0 2	

1513. C₈H₁₀N₂O₃S

Tosylurea

Tosyluree

RN: 1694-06-0**MP (°C):****MW:** 214.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.631E-03	7.779E-01	37	A028	1 0 2 1 2	intrinsic

1514. C₈H₁₀N₂O₄S

Asulam

Methyl N-(4-aminobenzenesulphonyl)carbamate

RN: 3337-71-1 MP (°C): 144

MW: 230.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.161E-02	4.975E+00	ns	M061	0 0 0 0 0	
2.188E-02	5.037E+00	ns	R427	0 0 0 0 0	
2.172E-02	5.000E+00	rt	M161	0 0 0 0 0	

1515. C₈H₁₀N₄O₂

Caffeine

Coffein

RN: 58-08-2 MP (°C): 238

MW: 194.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-02	7.548E+00	0	H023	1 0 2 1 2	
3.800E-02	7.379E+00	1	M116	2 1 1 1 1	
3.757E-02	7.296E+00	2	C074	1 0 0 1 2	
4.786E+00	9.294E+02	5	B429	1 0 1 2 2	
4.859E+00	9.436E+02	15	B429	1 0 1 2 2	
6.603E-02	1.282E+01	15	H023	1 0 2 1 2	
5.800E-02	1.126E+01	15	O017	1 0 1 1 1	
5.770E-02	1.121E+01	15	O018	1 2 1 1 2	
5.770E-02	1.121E+01	15	O019	1 0 0 1 2	
6.859E-02	1.332E+01	16	A072	1 0 1 0 2	
7.415E-02	1.440E+01	20	F300	1 0 0 0 2	
6.779E-02	1.316E+01	20	J009	2 0 2 2 2	
1.242E-01	2.411E+01	25	A068	2 0 0 0 2	
4.931E+00	9.575E+02	25	B429	1 0 1 2 2	
1.066E-01	2.071E+01	25	E016	1 1 1 1 2	
1.081E-01	2.100E+01	25	F300	1 0 0 0 1	
1.080E-01	2.097E+01	25	L329	2 2 1 2 2	
1.110E-01	2.156E+01	25	M116	2 1 1 1 2	
1.244E-01	2.415E+01	25	M158	2 0 2 2 2	
1.000E-01	1.942E+01	25	O017	1 0 1 1 2	
1.002E-01	1.946E+01	25	O018	1 2 1 1 2	
1.098E-02	2.132E+00	25	O019	1 0 0 1 2	
1.272E-01	2.470E+01	25	O302	1 0 0 1 0	
1.107E-01	2.150E+01	25	P010	1 0 1 1 2	
1.123E-01	2.180E+01	25	P011	0 0 0 0 0	
1.195E-01	2.320E+01	25	P018	1 0 2 2 2	
1.081E-01	2.100E+01	25	P020	2 0 1 1 1	
1.330E-01	2.583E+01	30	B042	1 2 1 1 2	
1.330E-01	2.583E+01	30	G021	1 0 0 0 2	
1.330E-01	2.583E+01	30	H020	1 0 0 0 2	
1.333E-01	2.589E+01	30	H023	1 0 2 1 2	

(continued)

1515. C₈H₁₀N₄O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-01	2.583E+01	30.60	M116	2 1 1 1 2	
4.999E+00	9.707E+02	35	B429	1 0 1 2 2	
1.670E-01	3.243E+01	35	O017	1 0 1 1 2	
1.909E-01	3.707E+01	37	C074	1 0 0 1 2	
1.930E-01	3.748E+01	37	M116	2 1 1 1 2	
5.041E+00	9.789E+02	40	B429	1 0 1 2 2	
2.266E-01	4.400E+01	40	F300	1 0 0 0 1	
5.211E-01	1.012E+02	57	C074	1 0 0 1 2	
1.408E+00	2.735E+02	83	C065	1 0 0 1 2	
1.407E+00	2.733E+02	85	C074	1 0 0 1 2	
1.739E+00	3.377E+02	87	C065	1 0 0 1 2	
2.343E+00	4.550E+02	90	C074	1 0 0 1 2	
1.287E-01	2.500E+01	ns	D035	0 0 0 0 2	
1.104E-01	2.143E+01	rt	D021	0 0 1 1 2	
1.596E-04	3.100E-02	rt	N015	0 0 2 2 1	<i>sic</i>
4.892E-02	9.500E+00	rt	R431	0 0 0 0 0	Average

1516. C₈H₁₀N₄O₂.H₂O

Caffeine (monohydrate)

1H-Purine-2,6-dione, 3,7-dihydro-1,3,7-trimethyl-, monohydrate

RN: 5743-12-4 MP (°C): 178

MW: 212.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.011E-01	2.146E+01	25	D004	0 0 0 0 0	

1517. C₈H₁₀N₄O₃

1,3,7-Trimethyluric acid

8-Oxy-caffeine

RN: 5415-44-1 MP (°C): 374

MW: 210.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-04	2.400E-02	rt	N015	0 0 2 2 1	

1518. C₈H₁₀O

4-Ethylphenol

p-Ethylphenol

RN: 123-07-9

MP (°C): 43.5

MW: 122.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.854E-02	5.931E+00	20	R087	0 0 0 0 0	0.15M NaCl
2.332E-02	2.849E+00	25	L022	1 0 0 0 0	
4.011E-02	4.900E+00	25	M127	1 0 0 0 1	
4.072E-02	4.975E+00	25	R041	0 0 0 0 0	
4.467E-02	5.457E+00	ns	R427	0 0 0 0 0	

1519. C₈H₁₀O

2,3-Xylenol

2,3-Dimethylphenol

RN: 526-75-0

MP (°C): 75

MW: 122.17

BP (°C): 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.740E-02	4.569E+00	25	A021	1 2 1 1 2	

1520. C₈H₁₀O

Phenylethylalcohol

Phenyl ethyl alcohol

RN: 60-12-8

MP (°C):

MW: 122.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-01	1.796E+01	20	S006	1 0 0 0 2	
1.720E-01	2.101E+01	25	D407	1 0 2 2 2	
1.432E-01	1.749E+01	25	H044	1 0 2 1 2	
1.455E-01	1.778E+01	30	H044	1 0 2 1 2	
1.487E-01	1.816E+01	35	H044	1 0 2 1 2	
1.518E-01	1.855E+01	40	H044	1 0 2 1 2	
1.542E-01	1.884E+01	45	H044	1 0 2 1 2	
1.562E-01	1.908E+01	50	H044	1 0 2 1 2	
1.597E-01	1.951E+01	55	H044	1 0 2 1 2	

1521. C₈H₁₀O

Phloral

RN:

MP (°C):

MW: 122.17

BP (°C): 204.52

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.072E-02	4.975E+00	25	L022	1 0 0 0 0	

1522. C₈H₁₀O

2,6-Xylenol
1,3,2-Xylenol
2,6-Dimethylphenol
Vic-*m*-xylenol

RN: 576-26-1 **MP (°C):** 49
MW: 122.17 **BP (°C):** 203

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.595E-02	4.392E+00	20	R087	0 0 0 0 0	0.15M NaCl
4.950E-02	6.047E+00	25	A021	1 2 1 1 2	
5.100E-02	6.231E+00	25	B316	0 0 0 0 0	

1523. C₈H₁₀O

2,4-Xylenol
2,4-Dimethylphenol
m-Xylenol
2,4-Dimethyl-phenol-
Phenol, 2,4-dimethyl-
1-Hydroxy-2,4-dimethylbenzene

RN: 105-67-9 **MP (°C):** 26
MW: 122.17 **BP (°C):** 211.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-02	5.375E+00	20	K132	1 0 1 1 1	
4.300E-02	5.253E+00	20	K309	1 0 0 1 1	
5.271E-02	6.440E+00	20	R087	0 0 0 0 0	0.15M NaCl
5.100E-02	6.231E+00	25	A021	1 2 1 1 2	
6.440E-02	7.868E+00	25	B173	2 0 2 2 2	
7.200E-02	8.796E+00	25	B316	0 0 0 0 0	
6.499E-02	7.940E+00	25	M127	1 0 0 0 2	
2.190E-01	2.675E+01	80	K309	1 0 0 1 2	

1524. C₈H₁₀O

α-Methyl-benzenemethanol
α-Methylbenzyl alcohol
1-Phenylethan-1-*o*
Methylphenylcarbinol
β-Hydroxyethylbenzene
(S)-1-Phenylethyl alcohol

RN: 98-85-1 **MP (°C):** 20
MW: 122.17 **BP (°C):** 401 at 0 mm

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.898E+00	8.427E+02	14.57	L441	0 0 0 0 0	
6.860E+00	8.380E+02	19.84	L441	0 0 0 0 0	

(continued)

1524. C₈H₁₀O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.056E-01	6.177E+01	92.71	L441	0 0 0 0 0	
6.491E+00	7.930E+02	94.89	L441	0 0 0 0 0	
6.445E+00	7.874E+02	105.95	L441	0 0 0 0 0	
6.196E+00	7.569E+02	127.92	L441	0 0 0 0 0	

1525. C₈H₁₀O

Phenetole

Ethoxybenzene

RN: 103-73-1 MP (°C): -30
 MW: 122.17 BP (°C): 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-03	5.498E-01	25	M327	1 0 0 1 2	
4.657E-03	5.690E-01	25.04	V013	2 2 2 2 2	

1526. C₈H₁₀O

2,5-Xylenol

2,5-Dimethylphenol

p-Xylenol

2,5-Dimethyl-phenol-

Phenol, 2,5-dimethyl-

RN: 95-87-4 MP (°C): 75
 MW: 122.17 BP (°C): 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-02	3.543E+00	25	A021	1 2 1 1 2	
2.600E-02	3.176E+00	25	B316	0 0 0 0 0	

1527. C₈H₁₀O

4-Methylbenzyl alcohol

4-Methyl-benzylalkohol

RN: 589-18-4 MP (°C): 60
 MW: 122.17 BP (°C): 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-02	8.430E+00	20	B407	1 0 1 2 2	

1528. C₈H₁₀O

3,4-Xylenol
3,4-Dimethylphenol
As-*o*-xylenol

RN: 95-65-8 **MP (°C):** 62.5
MW: 122.17 **BP (°C):** 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	3.787E+00	20	K132	1 0 1 1 1	
3.900E-02	4.765E+00	25	A021	1 2 1 1 2	
4.072E-02	4.975E+00	25	R041	0 0 0 0 0	
2.530E-02	3.091E+00	37	E028	1 0 1 1 2	

1529. C₈H₁₀O

3,5-Xylenol
3,5-Dimethylphenol

RN: 108-68-9 **MP (°C):** 64
MW: 122.17 **BP (°C):** 219.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-02	4.032E+00	20	K132	1 0 1 1 1	
2.961E-02	3.618E+00	20	R087	0 0 0 0 0	0.15M NaCl
4.000E-02	4.887E+00	25	A021	1 2 1 1 2	
4.000E-02	4.887E+00	25	B316	0 0 0 0 0	
3.981E-02	4.864E+00	ns	R427	0 0 0 0 0	

1530. C₈H₁₀O₂

o-Ethoxyphenol
2-Ethoxyphenol

RN: 94-71-3 **MP (°C):**
MW: 138.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.090E-02	8.414E+00	24.99	B353	0 0 0 0 0	

1531. C₈H₁₀O₂

Veratrole
o-Dimethoxybenzene

RN: 91-16-7 **MP (°C):** 15
MW: 138.17 **BP (°C):** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.842E-02	6.690E+00	25	L348	1 2 2 1 2	

1532. C₈H₁₀O₂

1,3-Dimethoxybenzene

m-Dimethoxybenzene

Dimethylresorcinol

RN: 151-10-0

MP (°C):

MW: 138.17

BP (°C): 86

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.800E-03	1.216E+00	25	M327	1 0 0 1 2	

1533. C₈H₁₀O₂

2-Phenoxyethanol

Phenoxyethyl alcohol

Ethylene glycol phenyl ether

Arosol

1-Hydroxy-2-phenoxyethane

Phenoxyethol

RN: 122-99-6

MP (°C): 12

MW: 138.17

BP (°C): 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.882E-01	2.601E+01	20	M062	1 0 0 0 2	
2.610E-01	3.606E+01	37	E028	1 0 1 1 2	

1534. C₈H₁₀O₂

3-Ethoxyphenol

m-Ethoxy phenol

Resorcinol monoethyl ether

RN: 621-34-1

MP (°C):

MW: 138.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-01	1.382E+01	25	B314	0 0 0 0 0	
1.003E-01	1.386E+01	30	B315	0 0 0 0 0	

1535. C₈H₁₀O₂*p*-Ethoxyphenol

Hydroquinone monoethyl ether

RN: 622-62-8

MP (°C): 64.5–67.5

MW: 138.17

BP (°C): 131 at 9 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.097E-02	7.043E+00	20	R087	0 0 0 0 0	0.15M NaCl

1536. C₈H₁₀O₂*p*-Dimethoxybenzene

4-Dimethoxybenzene

RN: 150-78-7

MP (°C):

MW: 138.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.530E-05	7.641E-03	25	C316	0 0 0 0 0	0.1M NaCl

1537. C₈H₁₀O₃

1,3-Dimethyl ether pyrogallol

Pyrogallol-1,3-dimethylaether

2,6-Dimethoxyphenol

RN: 91-10-1

MP (°C): 56

MW: 154.17

BP (°C): 262

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.116E-01	1.720E+01	13	F300	1 0 0 0 2	

1538. C₈H₁₀O₃S

Benzene sulfonic acid ethyl ester

Ethyl benzenesulfonate

Ethyl phenylsulfonate

RN: 515-46-8

MP (°C):

MW: 186.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.390E-03	1.376E+00	25	K097	2 0 2 2 2	

1539. C₈H₁₀O₄

Cyclohexene-1,4-dicarboxylic acid

Cyclohexen-(1)-dicarbonsaeure-(1,4)

RN: 2205-27-8

MP (°C): 312

MW: 170.17

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.175E-03	2.000E-01	20	F300	1 0 0 0 0	

1540. C₈H₁₀O₄

2-Cyclohexene-1,2-dicarboxylic acid

Cyclohexen-(2)-dicarbonsaeure-(1,2)

RN: 38765-78-5 MP (°C):

MW: 170.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.113E-02	8.700E+00	10	F300	1 0 0 0 1	

1541. C₈H₁₀O₅

Endothall

Endothal

RN: 145-73-3 MP (°C): 144

MW: 186.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.883E-01	9.091E+01	20	B200	1 0 0 0 2	
5.372E-01	1.000E+02	20	M161	1 0 0 0 2	
4.883E-01	9.091E+01	ns	B100	0 0 0 0 0	
4.883E-01	9.091E+01	ns	C307	0 0 0 0 1	

1542. C₈H₁₀O₈

meso-1,2,3,4-Butanetetracarboxylic acid

1,2,3,4-Butanetetracarboxylic acid

Butanetetracarboxylic acid

1,2,3,4-Butane tetracarboxylic acid

RN: 1703-58-8 MP (°C): 196

MW: 234.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.606E-01	1.547E+02	25	M370	1 2 2 1 2	

1543. C₈H₁₁BrN₂O₂

Isocil

Uracil, 5-bromo-3-isopropyl-6-methyl-

RN: 314-42-1 MP (°C): 158–159

MW: 247.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.701E-03	2.150E+00	25	B185	0 0 0 0 0	

1544. C₈H₁₁Cl₂NO*N,N*-Diallyldichloroacetamide

Dichlormid

N,N-Diallyl dichloroacetamide2,2-Dichloro-*N,N*-di-2-propenylacetamide

R 25788

RN: 37764-25-3 **MP (°C):** 5**MW:** 208.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.403E-02	5.000E+00	20	M161	1 0 0 0 0	
2.399E-02	4.992E+00	ns	S460	0 0 0 0 0	

1545. C₈H₁₁Cl₃O₆

Chloralose

1,2-*O*-(2,2,2-Trichloroethylidene)- α -D-glucofuranose

Anhydroglucochloral

Alfamat

Aphosal

Murex

RN: 15879-93-3 **MP (°C):** 187**MW:** 309.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.434E-02	4.440E+00	15	M161	1 0 0 0 2	

1546. C₈H₁₁N

Xylidine

N,N-Dimethylaniline

Dimethylaminobenzene

Benzanamine

Aminodimethylbenzene

RN: 121-69-7 **MP (°C):** 2**MW:** 121.18 **BP (°C):** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.120E-03	1.105E+00	25	C113	1 0 2 1 2	

1547. C₈H₁₁NO

Tyramine

Tyramin

4-Hydroxyphenylethylamine

4-(2-Aminoethyl)phenol

2-(*p*-Hydroxyphenyl)ethylamine**RN:** 51-67-2 **MP (°C):** 164.5**MW:** 137.18 **BP (°C):** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.574E-02	1.039E+01	15	D041	1 0 0 0 2	
7.581E-02	1.040E+01	15	F300	1 0 0 0 2	

1548. C₈H₁₁NO

Phenylethanolamine

Phenyl ethanolamine

2-Anilinoethanol

β-Hydroxyethyl aniline

N-Phenylethanolamine

PEA

RN: 7568-93-6 **MP (°C):** 56.5**MW:** 137.18 **BP (°C):** 286.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.192E-01	4.379E+01	20	M062	1 0 0 0 2	

1549. C₈H₁₁N₂O₅PS

Parathion-amino

Aminoparathion

RN: **MP (°C):****MW:** 278.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.419E-03	3.948E-01	19.50	B169	2 2 1 1 2	

1550. C₈H₁₁N₃O₃S

Lamivudine

2(1H)-Pyrimidinone,4-amino-1-[2-(hydroxymethyl)-1,3-oxathiolan-5-yl]-,(2R-*cis*)

Epivir

3'-Thia-2',3'-dideoxycytidine

(-)NGPB-21

(-) 2'-Deoxy-3'-thiacytidine

RN: 134678-17-4 **MP (°C):****MW:** 229.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.053E-01	7.000E+01	ns	K444	0 0 0 0 0	
3.053E-01	7.000E+01	rt	B435	0 0 0 0 0	

1551. C₈H₁₁N₅O₃

Acyclovir

Acycloguanosine

9-(2-Hydroxyethoxymethyl)guanine

6H-Purin-6-one, 2-amino-1,9-dihydro-9-[(2-hydroxyethoxy)methyl]-

Cargosil

Zovirax

RN: 59277-89-3 **MP (°C):****MW:** 225.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.216E-03	1.400E+00	21	B419	1 1 2 2 1	int
7.150E-03	1.610E+00	22	K443	0 0 0 0 0	
7.244E-03	1.631E+00	22	K445	0 0 0 0 0	
5.380E-03	1.212E+00	22.5	B422	2 0 2 2 2	
2.240E+00	5.045E+02	25	B443	0 0 0 0 0	
8.070E-03	1.817E+00	25	Z407	0 0 0 0 0	
4.440E-02	1.000E+01	ns	K444	0 0 0 0 0	
6.166E-03	1.389E+00	ns	R427	0 0 0 0 0	

1552. C₈H₁₂

4-Vinylcyclohexene

4-Vinyl-1-cyclohexene

RN: 100-40-3 **MP (°C):** -101**MW:** 108.18 **BP (°C):** 145

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.622E-04	5.000E-02	25	M001	2 1 2 2 1	

1553. C₈H₁₂ClNO

Allidochlor

CDAA

N,N-Diallyl-2-chloroacetamide

Rodox

2-Chloro-N,N-diallylacetamide

CP 6343

RN: 93-71-0 **MP (°C):****MW:** 173.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.113E-01	1.932E+01	22	J008	1 0 0 0 2	
1.113E-01	1.932E+01	25	B185	0 0 0 0 0	
1.135E-01	1.970E+01	25	G319	0 0 0 0 0	
1.135E-01	1.970E+01	25	M161	1 0 0 0 2	
1.129E-01	1.961E+01	ns	B100	0 0 0 0 0	
1.130E-01	1.962E+01	ns	F184	0 0 0 0 2	
1.129E-01	1.961E+01	ns	M061	0 0 0 0 0	
3.162E-01	5.491E+01	ns	M163	0 0 0 0 0	EFG

1554. C₈H₁₂N₂O₂S

N1-Dimethylsulfanilamide

p-Amino-*N,N*-dimethylbenzenesulfonamide

[(4-Aminophenyl)sulfonyl]dimethylamine

p-(Dimethylsulfamoyl)aniline

RN: 1709-59-7 MP (°C):

MW: 200.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.130E-03	6.268E-01	37	K095	2 0 0 0 2	intrinsic

1555. C₈H₁₂N₂O₂S

5,5-Diethyl-2-thiobarbituric acid

4,6(1H,5H)-Pyrimidinedione, 5,5-diethyldihydro-2-thioxo

Barbituric acid, 5,5-diethyl-2-thio

Certodorm

RN: 77-32-7 MP (°C):

MW: 200.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.810E-03	1.364E+00	25	P350	0 0 0 0 0	intrinsic

1556. C₈H₁₂N₂O₃

Barbital

5,5-Diethylbarbituric acid

Diethylmalonylurea

RN: 57-44-3 MP (°C): 190

MW: 184.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	3.131E+00	0	M143	1 2 1 1 0	
1.900E-02	3.500E+00	0	M143	1 2 1 1 2	
2.562E-02	4.720E+00	10	N007	1 2 2 2 2	form I
1.900E-02	3.500E+00	10	N007	1 2 2 2 2	form III
3.100E-02	5.710E+00	14	I006	1 0 0 0 1	
3.187E-02	5.870E+00	15	H018	0 0 0 0 0	
3.500E-02	6.447E+00	19	I006	1 0 0 0 1	
4.522E-02	8.330E+00	20	D041	1 0 0 0 1	
3.637E-02	6.700E+00	20	F300	1 0 0 0 1	
3.415E-02	6.290E+00	20	J030	1 2 2 2 2	
2.839E-02	5.230E+00	20	N007	1 2 2 2 2	form III
3.409E-02	6.280E+00	20	N007	1 2 2 2 2	form I
3.806E-02	7.011E+00	20	S146	2 2 2 1 2	form I
3.752E-02	6.912E+00	20	S146	2 2 2 1 2	form II
3.881E-02	7.149E+00	25	A023	1 0 0 1 2	
3.963E-02	7.300E+00	25	B011	2 0 0 1 0	
3.971E-02	7.314E+00	25	B065	1 1 1 1 1	
3.746E-02	6.900E+00	25	B167	1 1 0 0 1	pH 5.7 (continued)

1556. C₈H₁₂N₂O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.860E-02	7.110E+00	25	G003	1 1 1 1 2	pH 4.7
2.800E-02	5.158E+00	25	M143	1 2 1 1 2	
4.050E-02	7.460E+00	25	M310	2 2 2 2 2	
4.018E-02	7.401E+00	25	P350	0 0 0 0 0	intrinsic
4.239E-02	7.809E+00	25	S146	2 2 2 1 2	form II
4.010E-03	7.386E-01	25	V033	2 0 1 1 2	
4.010E-02	7.386E+00	25.00	T303	1 0 0 0 2	
4.300E-02	7.920E+00	27	I006	1 0 0 0 1	
4.300E-02	7.920E+00	30	G014	1 1 1 1 0	EFG, 0.003N H ₂ SO ₄
2.704E-02	4.980E+00	30	H005	1 0 1 2 2	average of 4
4.408E-02	8.119E+00	30	H018	0 0 0 0 0	
4.400E-02	8.105E+00	30	I001	2 0 2 1 0	EFG, 0.003N H ₂ SO ₄
4.260E-02	7.847E+00	30	K108	1 2 2 0 2	
4.425E-02	8.150E+00	30	N007	1 2 2 2 2	form I
4.207E-02	7.750E+00	30	N007	1 2 2 2 2	form III
4.720E-02	8.694E+00	30	S146	2 2 2 1 2	form I
4.618E-02	8.507E+00	30	S146	2 2 2 1 2	form II
5.162E-02	9.509E+00	35	S146	2 2 2 1 2	form I
5.184E-02	9.548E+00	35	S146	2 2 2 1 2	form II
5.150E-02	9.486E+00	35.00	T303	1 0 0 0 2	
4.843E-02	8.920E+00	36	A023	1 0 0 1 2	
5.152E-02	9.490E+00	37	J030	1 2 2 2 2	
5.300E-02	9.762E+00	37	K121	1 2 1 2 1	0.1N HCl
5.538E-02	1.020E+01	37	N007	1 2 2 2 2	form III
5.277E-02	9.720E+00	37	N007	1 2 2 2 2	form I
5.668E-02	1.044E+01	37	S146	2 2 2 1 2	form II
5.588E-02	1.029E+01	40	A023	1 0 0 1 1	
6.100E-01	1.124E+02	40	N008	1 0 1 1 2	sic
6.967E-02	1.283E+01	45	S146	2 2 2 1 2	form II
6.800E-02	1.253E+01	45.00	T303	1 0 0 0 2	
4.343E-01	8.000E+01	100	F300	1 0 0 0 1	
3.257E-02	6.000E+00	ns	T003	0 0 0 0 2	

1557. C₈H₁₂O₂

1-Epoxyethyl-3,4-epoxycyclohexane

Vinylcyclohexene dioxide

RN: 106-87-6 MP (°C): <-55

MW: 140.18 BP (°C): 227

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.103E+00	1.547E+02	20	I313	0 0 0 0 0	

1558. C₈H₁₂O₄

trans-Cyclohexane-1,2-dicarboxylic acid
trans-Cyclohexan-dicarbonsaeure-(1,2)

RN: 2305-32-0 MP (°C):
 MW: 172.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.162E-02	2.000E+000	20	F300	1 0 0 0 0	

1559. C₈H₁₂O₄

cis-Cyclohexane-1,2-dicarboxylic acid
cis-Cyclohexan-dicarbonsaeure-(1,2)
 RN: 610-09-3 MP (°C): 193
 MW: 172.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.16E-02	>2.00E+000	20	F300	1 0 0 0 0	

1560. C₈H₁₂O₄

trans-Cyclohexane-1,4-dicarboxylic acid
trans-Cyclohexan-dicarbonsaeure-(1,4)
 RN: 619-82-9 MP (°C):
 MW: 172.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.646E-03	8.000E-01	17	F300	1 0 0 0 0	
7.550E-02	1.300E+01	100	F300	1 0 0 0 1	

1561. C₈H₁₃BrN₂O₂

α-Bromethylpropylaceturea
 RN: MP (°C):
 MW: 249.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.645E-03	4.098E-01	20	O021	1 0 0 0 0	

1562. C₈H₁₃NO

Diaallylacetamide
 α,α-Diallylacetamide
 2-(2-Propenyl)4-pentenamide
 RN: 60730-94-1 MP (°C):
 MW: 139.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-01	1.750E+01	ns	H348	0 0 0 0 0	

1563. C₈H₁₃N₂O₃PS

Thionazin

O,O-Diethyl O-pyrazinyl thiophosphate

RN: 297-97-2 **MP (°C):** -1.7
MW: 248.24 **BP (°C):** 80

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	1.140E+00	25	M061	1 0 0 0 2	
4.592E-03	1.140E+00	27	M161	1 0 0 0 2	

1564. C₈H₁₄

1-Octyne

Hexylacetylene

n-Hexylacetylene

RN: 629-05-0 **MP (°C):** -80
MW: 110.20 **BP (°C):** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.178E-04	2.400E-02	25	M001	2 1 2 2 2	

1565. C₈H₁₄

2,2-Dimethyl-3-hexyne

1-Ethyl-2-tertbutylacetylene

RN: 4911-60-8 **MP (°C):**
MW: 110.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-04	7.934E-02	25	H039	1 2 2 2 1	

1566. C₈H₁₄ClNS₂

Carbamic acid, diethyldithio-2chloroallyl ester

2-Chloroallyl diethyldithiocarbamate

CDEC

RN: 95-06-7 **MP (°C):** <25
MW: 223.79 **BP (°C):** 128

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.469E-04	1.000E-01	25	B185	0 0 0 0 0	
4.111E-04	9.200E-02	25	B200	1 0 0 0 1	
4.469E-04	1.000E-01	25	F019	1 0 0 0 2	
4.111E-04	9.200E-02	25	G319	0 0 0 0 0	
4.111E-04	9.200E-02	25	M161	1 0 0 0 1	
4.468E-04	9.999E-02	ns	M061	0 0 0 0 0	approximate

1567. C₈H₁₄ClN₅

Atrazine

2-Chloro-4-ethylamino-6-isopropylamino-*s*-triazine

RN: 1912-24-9 MP (°C): 172

MW: 215.69 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-04	2.200E-02	0	B185	0 0 0 0 0	
1.390E-04	2.998E-02	1	G091	1 0 1 2 2	pH 6.0
5.000E-04	1.078E-01	2	B193	1 2 0 0 0	
1.410E-04	3.041E-02	8	G091	1 0 1 2 2	pH 6.0
1.530E-04	3.300E-02	20	A314	0 0 0 0 0	
1.345E-04	2.900E-02	20	C048	2 2 2 2 1	
1.391E-04	3.000E-02	20	E048	1 2 1 1 1	
1.391E-04	3.000E-02	20	F311	1 2 2 2 1	
1.580E-04	3.408E-02	20	G091	1 0 1 2 2	pH 6.0
1.298E-04	2.800E-02	20	M161	1 0 0 0 1	
1.391E-04	3.000E-02	20	N333	0 0 0 0 0	
3.245E-04	7.000E-02	21	B192	0 0 0 0 1	
3.245E-04	7.000E-02	21	G099	2 0 0 1 0	
3.245E-04	7.000E-02	22	M061	1 0 0 0 1	
1.530E-04	3.300E-02	25	H024	2 2 2 2 2	
1.386E-04	2.990E-02	25	H073	2 1 1 2 2	
1.530E-04	3.300E-02	25	P434	0 0 0 0 0	
3.245E-04	7.000E-02	27	B185	0 0 0 0 0	
1.530E-04	3.300E-02	27	B200	1 0 0 0 1	
1.970E-04	4.249E-02	29	G091	1 0 1 2 2	pH 6.0
4.530E-04	9.771E-02	50	G001	1 0 0 1 2	
1.484E-03	3.200E-01	85	B185	0 0 0 0 0	
3.245E-04	7.000E-02	ns	C101	0 0 0 0 1	
3.245E-04	7.000E-02	ns	G041	0 0 0 0 1	
3.245E-04	7.000E-02	ns	H112	0 0 0 0 1	
1.530E-04	3.300E-02	ns	J033	0 0 0 0 0	
3.941E-04	8.500E-02	ns	M110	0 0 0 0 0	EFG
1.609E-04	3.470E-02	ns	V414	0 0 0 0 0	

1568. C₈H₁₄N₂O₂

cis-N,N,N',N'-Tetramethylfumaramide

2-Butenediamide, N,N,N',N'-tetramethyl-, (Z)-

RN: 35075-35-5 MP (°C):

MW: 170.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E+00	2.945E+02	30	K019	1 0 0 0 2	

1569. C₈H₁₄N₄OS

Metribuzin

4-Amino-6-*tert*-butyl-3-(methylthio)-as-triazin-5(4H)-one

Bayer 6159H

Lexone

Sencor

Sencorex

RN: 21087-64-9 **MP (°C):** 125.8**MW:** 214.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-03	1.200E+00	20	M161	1 0 0 0 1	
5.693E-03	1.220E+00	22.5	G301	0 0 0 0 0	
4.662E-03	9.990E-01	ns	B100	0 0 0 0 0	
7.000E-03	1.500E+00	ns	M110	0 0 0 0 0	EFG

1570. C₈H₁₄O

Bicyclo[2.2.1]heptylcarbinol

2-Norcamphanemethanol

RN: 5240-72-2 **MP (°C):****MW:** 126.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.916E-03	9.990E-01	ns	M061	0 0 0 0 0	

1571. C₈H₁₄O₂

2,4-Octadione

Valeryacetone

RN: 14090-87-0 **MP (°C):****MW:** 142.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-02	3.925E+00	25	M078	2 0 1 0 2	

1572. C₈H₁₄O₂

Cyclohexanol acetate

Hexalin acetate

Cyclohexyl acetate

RN: 622-45-7 **MP (°C):** <25**MW:** 142.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.123E-02	1.597E+00	20	D052	1 1 0 0 1	
2.033E-02	2.892E+00	23.50	O005	2 0 2 2 1	
2.138E-02	3.040E+00	ns	S460	0 0 0 0 0	

1573. C₈H₁₄O₂

6-Methyl-2,4-heptadione
 2-Methyl-4,6-heptanedione
 Isovalerylacetone

RN: 3002-23-1 **MP (°C):** <25
MW: 142.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.490E-02	3.541E+00	25	M078	2 0 1 0 2	

1574. C₈H₁₄O₂

3-Propyl-2,4-pentadione
 3-Acetyl-2-hexanone

RN: 1540-35-8 **MP (°C):** <25
MW: 142.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-01	1.891E+01	25	M078	2 0 1 0 2	

1575. C₈H₁₄O₂

5,5-Dimethyl-2,4-hexadione
 Pivaloylacetone
 Pivaloylacetyl methane

RN: 7307-04-2 **MP (°C):**
MW: 142.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.340E-02	3.327E+00	25	M078	2 0 1 0 2	

1576. C₈H₁₄O₂S₄

Propyl dixanthogen
 bis(1-Propyl) dixanthogen
 Propyl xanthogen disulfide
 Dipropyl dixanthogen
 Dipropyl thioperoxydicarbonate
 Dipropyl xanthogen disulfide

RN: 3750-28-5 **MP (°C):**
MW: 270.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-06	4.057E-04	25	H102	1 2 1 2 1	

1577. C₈H₁₄O₄

Suberic acid

Korksaeure

RN: 505-48-6 **MP (°C):** 142
MW: 174.20 **BP (°C):** 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	8.000E-01	0	L041	1 0 0 1 0	
5.301E-03	9.234E-01	6.99	A340	0 0 0 0 0	
7.097E-03	1.236E+00	12.69	A340	0 0 0 0 0	
8.037E-03	1.400E+00	15	F300	1 0 0 0 1	
7.463E-03	1.300E+00	15	L041	1 0 0 1 1	
7.463E-03	1.300E+00	15	M051	1 0 0 0 1	
9.789E-03	1.705E+00	18.69	A340	0 0 0 0 0	
9.185E-03	1.600E+00	20	L041	1 0 0 1 1	
8.986E-03	1.565E+00	20	M171	1 0 0 0 0	
1.206E-01	2.100E+01	21	B040	1 0 1 1 2	<i>sic</i>
1.388E-02	2.417E+00	24.99	A340	0 0 0 0 0	
3.387E-02	5.900E+00	25	F300	1 0 0 0 1	
6.800E-02	1.185E+01	25	K040	1 0 2 1 2	<i>sic</i>
1.700E-02	2.961E+00	30	H021	1 0 1 1 0	EFG
1.890E-02	3.293E+00	32.49	A340	0 0 0 0 0	
2.045E-02	3.563E+00	34.49	A340	0 0 0 0 0	
2.583E-02	4.500E+00	35	L041	1 0 0 1 1	
2.326E-02	4.051E+00	39.99	A340	0 0 0 0 0	
2.682E-02	4.673E+00	44.49	A340	0 0 0 0 0	
5.626E-02	9.800E+00	50	L041	1 0 0 1 1	
3.198E-02	5.571E+00	50.19	A340	0 0 0 0 0	
3.534E-02	6.156E+00	52.69	A340	0 0 0 0 0	
5.551E-02	9.670E+00	61.49	A340	0 0 0 0 0	
6.422E-02	1.119E+01	63.99	A340	0 0 0 0 0	
1.274E-01	2.220E+01	65	L041	1 0 0 1 2	
8.182E-02	1.425E+01	70.09	A340	0 0 0 0 0	
1.156E-01	2.013E+01	76.49	A340	0 0 0 0 0	
1.386E-02	2.414E+00	rt	H431	0 0 0 0 0	

1578. C₈H₁₄O₄

Diethyl succinate

Butanedioic acid, diethyl ester

RN: 123-25-1 **MP (°C):** -20
MW: 174.20 **BP (°C):** 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.089E-02	1.896E+00	ns	F014	0 0 0 0 2	

1579. C₈H₁₄O₄

Butylene glycol diacetate
1,4-Diacetoxybutane
Tetramethylene acetate

RN: 628-67-1 **MP (°C):**
MW: 174.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.005E-01	3.494E+01	26	O012	1 2 1 1 2	
1.602E-01	2.790E+01	50	O012	1 2 1 1 2	
2.048E-01	3.568E+01	75	O012	1 2 1 1 2	

1580. C₈H₁₄O₄

Tetramethyl succinic acid
Tetramethyl-bernsteinsaeure

RN: 630-51-3 **MP (°C):**
MW: 174.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.755E-02	4.800E+00	13.5	F300	1 0 0 0 1	

1581. C₈H₁₄O₄

Isoamylmalonic acid
Acide isoamylmalonique

RN: 616-87-5 **MP (°C):**
MW: 174.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E+00	3.850E+02	0	M051	1 0 0 0 2	
2.974E+00	5.180E+02	15	M051	1 0 0 0 2	
3.490E+00	6.080E+02	25	M051	1 0 0 0 2	
4.788E+00	8.340E+02	50	M051	1 0 0 0 2	

1582. C₈H₁₄O₄

Propyl α -acetoxypropionate
Hydracrylic acid, propyl ester, acetate

RN: 20473-73-8 **MP (°C):**
MW: 174.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.683E-02	9.900E+00	25	R006	2 2 0 1 1	

1583. C₈H₁₄O₄

Ethylene glycol dipropionate
 1,2-Ethanediol, dipropanoate
 1,2-bis(Propionyloxy)ethane

RN: 123-80-8 **MP (°C):**
MW: 174.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.480E-02	1.651E+01	25	F064	1 0 0 0 2	
9.170E-03	1.597E+00	ns	F014	0 0 0 0 2	

1584. C₈H₁₄O₅

Propanoic acid, 2-[(propoxycarbonyl)oxy]-, methyl ester

RN: **MP (°C):**
MW: 190.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-02	5.173E+00	25	R007	0 0 0 0 0	

1585. C₈H₁₅CIN₅O

Hydroxyatrazine

4-(Ethylamino)-6-[(1-methylethyl)amino]-1,3,5-triazin-2(1H)-one

2-Hydroxy atrazine

RN: 2163-68-0 **MP (°C):**
MW: 232.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.585E-02	2	B193	1 2 0 0 1	

1586. C₈H₁₅NO

Pelletierine

Pelletierin

RN: 2858-66-4 **MP (°C):** <25
MW: 141.21 **BP (°C):** 195

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.541E-01	5.000E+01	20	F300	1 0 0 0 0	
3.372E-01	4.762E+01	25	D004	0 0 0 0 0	

1587. C₈H₁₅NO

Propylallylacetamide

2-Propyl-4-pentenamide

PAD

RN: 90204-40-3 MP (°C):

MW: 141.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.727E-02	9.500E+00	37	H347	0 0 0 0 0	

1588. C₈H₁₅NO₂S

4-Thiazolidinecarboxylic acid, 2-butyl-

RN: 90205-28-0 MP (°C):

MW: 189.28 BP (°C): 355.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	1.079E+01	21	B414	1 0 0 1 1	partial decomposition

1589. C₈H₁₅NO₂S

4-Thiazolidinecarboxylic acid, 2-(2-methylpropyl)-

4-Thiazolidine-4-carboxylic acid, 2-(2-isobutyl)-

RN: 215669-71-9 MP (°C):

MW: 189.28 BP (°C): 347.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-02	9.275E+00	21	B414	1 0 0 1 1	partial decomposition

1590. C₈H₁₅N₃O₂

Isocarbamid

N-(2-Methylpropyl)-2-oxo-1-imidazolidinecarboxamide

RN: 30979-48-7 MP (°C): 95.5

MW: 185.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.018E-03	1.300E+00	20	M161	1 0 0 0 1	

1591. C₈H₁₅N₃O₇

Streptozotocin

Streptozocin

D-2-Deoxy-2-(3-methyl-3-nitrosoureido)glucopyranose

RN: 18883-66-4 **MP (°C):** 115**MW:** 265.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-02	5.066E+00	25	I307	0 0 0 0 0	

1592. C₈H₁₅N₅O

Simetone

2-Methoxy-4,6-bis(ethylamino)-*s*-triazine*s*-Triazole, 2,4-bis(ethylamine)-6-methoxy-**RN:** 673-04-1 **MP (°C):** 118-120**MW:** 197.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.622E-02	3.200E+00	21	B185	0 0 0 0 0	
1.622E-02	3.200E+00	21	B192	0 0 0 0 2	
1.622E-02	3.200E+00	21	G099	2 0 0 1 0	
3.550E-02	7.002E+00	50	G001	1 0 1 1 2	
1.622E-02	3.200E+00	ns	C101	0 0 0 0 1	

1593. C₈H₁₅N₅O2-Methoxy-4-methylamino-6-isopropylamino-*s*-triazine

Noratone

RN: 3035-45-8 **MP (°C):****MW:** 197.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.774E-02	3.500E+00	20	J033	0 0 0 0 0	
1.774E-02	3.500E+00	21	B192	0 0 0 0 2	

1594. C₈H₁₅N₅S

Desmetryne

N-Methyl-*N'*-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine

Semeron

Methylamino-4-methylthio-6-isopropylamino-1,3,5-triazine

Topusyn

Methylthio-4-isopropylamino-6-methylamino-*s*-triazine**RN:** 1014-69-3 **MP (°C):****MW:** 213.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E-03	6.000E-01	20	F311	1 2 2 2 1	
2.719E-03	5.800E-01	20	M161	1 0 0 0 2	
2.811E-03	5.996E-01	ns	B100	0 0 0 0 0	

(continued)

1594. C₈H₁₅N₅S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-03	5.800E-01	ns	J033	0 0 0 0 0	
2.719E-03	5.800E-01	ns	M061	0 0 0 0 2	

1595. C₈H₁₅N₅S

Simetryne

N,N'-Diethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine

G-32911

bis(Ethylamino)-6-(methylthio)-s-triazine

Methylthio-4,6-bis(ethylamino)-s-triazine

Cymetrin

RN: 1014-70-6 MP (°C): 82

MW: 213.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-03	1.003E+00	50	G001	1 0 1 1 1	
2.110E-03	4.500E-01	ns	C101	0 0 0 0 1	
2.110E-03	4.500E-01	ns	J033	0 0 0 0 0	
2.110E-03	4.500E-01	rt	M161	0 0 0 0 2	

1596. C₈H₁₅N₇O₂S₃

Famotidine

Amfamox

N'-(Aminosulfonyl)-3-(((2-((diaminomethylene)amino)-4-thiazolyl)methyl)thio)propanimidamide

Pepcid

Pepcidine

Pepcid PM

RN: 76824-35-6 MP (°C):

MW: 337.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.260E-06	1.100E-03	25	A408	2 0 1 2 0	
3.311E-03	1.117E+00	ns	R427	0 0 0 0 0	

1597. C₈H₁₆

Cyclooctane

RN: 292-64-8 MP (°C): 10

MW: 112.22 BP (°C): 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.619E-03	1.817E-01	20	M337	2 1 2 2 2	sic
7.040E-05	7.900E-03	25	M001	2 1 2 2 1	
7.040E-05	7.900E-03	ns	H123	0 0 0 0 0	

1598. C₈H₁₆

Caprylene

1-Octene

RN: 111-66-0 **MP (°C):** -102
MW: 112.22 **BP (°C):** 121.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E-05	3.600E-03	23	C332	0 0 0 0 0	
2.406E-05	2.700E-03	25	M001	2 1 2 2 1	
3.650E-05	4.096E-03	25	M342	1 0 1 1 2	

1599. C₈H₁₆

1,4-Dimethylcyclohexane

p-Dimethylcyclohexane

RN: 589-90-2 **MP (°C):** -87
MW: 112.22 **BP (°C):** 120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.422E-05	3.840E-03	25	K119	1 0 0 0 2	

1600. C₈H₁₆*cis*-1,2-Dimethylcyclohexane1-*cis*-2-Dimethylcyclohexane

RN: 2207-01-4 **MP (°C):** -50
MW: 112.22 **BP (°C):** 129

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.773E-05	7.600E-03	20	M337	2 1 2 2 1	
5.347E-05	6.000E-03	25	M001	2 1 2 2 1	

1601. C₈H₁₆*n*-Propylcyclopentane

1-Propylcyclopentane

RN: 2040-96-2 **MP (°C):** -117
MW: 112.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.818E-05	2.040E-03	25	K119	1 0 0 0 2	
1.818E-05	2.040E-03	25	P051	2 1 1 2 2	
1.818E-05	2.040E-03	25.00	P007	2 1 2 2 2	

1602. C₈H₁₆*trans*-1,2-Dimethylcyclohexane1,2-*trans*-Dimethylcyclohexane**RN:** 6876-23-9 **MP (°C):** -89**MW:** 112.22 **BP (°C):** 123

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.634E-05	5.200E-03	20	M337	2 1 2 2 1	
4.444E-05	4.987E-03	30.2	M447	0 0 0 0 0	
1.061E-04	1.191E-02	70.3	M447	0 0 0 0 0	
2.611E-04	2.930E-02	100.7	M447	0 0 0 0 0	
6.000E-04	6.733E-02	131.0	M447	0 0 0 0 0	
1.239E-03	1.390E-01	151.0	M447	0 0 0 0 0	
1.977E-03	2.219E-01	170.1	M447	0 0 0 0 0	

1603. C₈H₁₆*trans*-1,4-Dimethylcyclohexane

1,4-Transdimethylcyclohexane

RN: 2207-04-7 **MP (°C):** -37**MW:** 112.22 **BP (°C):** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.422E-05	3.840E-03	25	P051	2 1 1 2 2	
3.422E-05	3.840E-03	25.00	P007	2 1 2 2 2	

1604. C₈H₁₆1,2-Dimethylcyclohexane (*cis* + *trans*)Cyclohexane, 1,2-dimethyl- (*cis/trans*)

1,2-Dimethylcyclohexane

RN: 583-57-3 **MP (°C):****MW:** 112.22 **BP (°C):** 124 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.056E-05	6.795E-03	30.0	M447	0 0 0 0 0	
1.200E-04	1.347E-02	70.0	M447	0 0 0 0 0	
2.422E-04	2.718E-02	100.2	M447	0 0 0 0 0	
5.483E-04	6.153E-02	130.5	M447	0 0 0 0 0	
1.089E-03	1.222E-01	150.5	M447	0 0 0 0 0	
2.422E-03	2.717E-01	170.5	M447	0 0 0 0 0	

1605. C₈H₁₆

1,1,3-Trimethylcyclopentane

Cyclopentane, 1,1,3-trimethyl-

RN: 4516-69-2 MP (°C): -142.4

MW: 112.22 BP (°C): 104.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.324E-05	3.730E-03	25	K119	1 0 0 0 2	
3.324E-05	3.730E-03	25	P051	2 1 1 2 2	
3.324E-05	3.730E-03	25.00	P007	2 1 2 2 2	

1606. C₈H₁₆

Ethyl cyclohexane

Cyclohexane, ethyl-

RN: 1678-91-7 MP (°C):

MW: 112.22 BP (°C): 131.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
5.614E-05	6.300E-03	20	M337	2 1 2 2 1	
3.883E-05	4.358E-03	30.3	M447	0 0 0 0 0	
7.833E-05	8.790E-03	70.4	M447	0 0 0 0 0	
2.511E-04	2.818E-02	100.5	M447	0 0 0 0 0	
6.055E-04	6.795E-02	131.0	M447	0 0 0 0 0	
9.871E-04	1.108E-01	151.2	M447	0 0 0 0 0	
1.633E-03	1.833E-01	170.8	M447	0 0 0 0 0	

1607. C₈H₁₆Br₂

1,8-Dibromoocetane

Octamethylene dibromide

RN: 4549-32-0 MP (°C): 15–16

MW: 272.03 BP (°C): 270–272

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
7.389E-06	2.010E-03	1.0	S464	0 0 0 0 0	
7.278E-06	1.980E-03	1.0	S464	0 0 0 0 0	
7.462E-06	2.030E-03	4.9	S464	0 0 0 0 0	
7.646E-06	2.080E-03	4.9	S464	0 0 0 0 0	
8.565E-06	2.330E-03	10.0	S464	0 0 0 0 0	
8.896E-06	2.420E-03	14.9	S464	0 0 0 0 0	
8.528E-06	2.320E-03	14.9	S464	0 0 0 0 0	
9.374E-06	2.550E-03	19.9	S464	0 0 0 0 0	
1.062E-05	2.890E-03	25	S464	0 0 0 0 0	
1.066E-05	2.900E-03	25.0	S464	0 0 0 0 0	
1.044E-05	2.840E-03	25.0	S464	0 0 0 0 0	
1.209E-05	3.290E-03	30.0	S464	0 0 0 0 0	
1.239E-05	3.370E-03	30.0	S464	0 0 0 0 0	
1.213E-05	3.300E-03	30.1	S464	0 0 0 0 0	

(continued)

1607. C₈H₁₆Br₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.261E-05	3.430E-03	34.9	S464	0 0 0 0 0	
1.309E-05	3.560E-03	35.0	S464	0 0 0 0 0	
1.430E-05	3.890E-03	40.1	S464	0 0 0 0 0	
1.386E-05	3.770E-03	40.1	S464	0 0 0 0 0	

1608. C₈H₁₆Cl₂

1,8-Dichlorooctane

RN: 2162-99-4

MP (°C): -8

MW: 183.12

BP (°C): 243

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.441E-05	4.470E-03	3.6	S464	0 0 0 0 0	
3.047E-05	5.580E-03	5.1	S464	0 0 0 0 0	
3.014E-05	5.520E-03	5.1	S464	0 0 0 0 0	
3.069E-05	5.620E-03	9.9	S464	0 0 0 0 0	
3.233E-05	5.920E-03	15.1	S464	0 0 0 0 0	
3.211E-05	5.880E-03	25.1	S464	0 0 0 0 0	
3.255E-05	5.960E-03	25.1	S464	0 0 0 0 0	
3.222E-05	5.900E-03	25.1	S464	0 0 0 0 0	
3.517E-05	6.440E-03	30.3	S464	0 0 0 0 0	
3.375E-05	6.180E-03	30.3	S464	0 0 0 0 0	
3.823E-05	7.000E-03	35.2	S464	0 0 0 0 0	
3.828E-05	7.010E-03	35.3	S464	0 0 0 0 0	
3.970E-05	7.270E-03	40.1	S464	0 0 0 0 0	

1609. C₈H₁₆N₂O₂

N,N,N',N'-Tetramethylsuccinamide

N,N,N',N'-Tetramethylbutanediamide

RN: 7334-51-2

MP (°C):

MW: 172.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.188E+00	5.490E+02	30	K004	1 0 0 0 2	

1610. C₈H₁₆N₂O₄S₂

DL-Homocystine

DL-*meso*-Homocystine

Oxidized DL-homocysteine

RN: 870-93-9

MP (°C): 264

MW: 268.36

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.451E-04	2.000E-01	25	D041	1 0 0 0 0	

1611. C₈H₁₆N₆

Pentamethylmelamine

1-(Methylamino)-3,5-bis(dimethylamino)-*s*-triazine

RN: 16268-62-5 MP (°C): 107.0

MW: 196.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.679E-04	3.295E-02	25	B386	0 0 0 0 0	
1.010E-02	1.982E+00	25	B386	0 0 0 0 0	
1.101E-02	2.160E+00	25	C051	1 2 1 1 2	pH 7

1612. C₈H₁₆N₆O

N2-Hydroxy-N2,N4,N4,N6,N6-pentamethylmelamine

1-(Hydroxylamino)-3,5-bis(dimethylamino)-*s*-triazine

RN: 64124-14-7 MP (°C): 110.0

MW: 212.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.412E-03	9.365E-01	25	B386	0 0 0 0 0	
4.259E-03	9.040E-01	25	C051	1 2 1 1 2	pH 7

1613. C₈H₁₆O

Cyclooctanol

RN: 696-71-9 MP (°C): 15

MW: 128.22 BP (°C): 106–108 at 22 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.129E-02	6.576E+00	ns	S460	0 0 0 0 0	

1614. C₈H₁₆O

1-Octen-3-ol

3-Octenol

Flowtron mosquito attractant

Matsuka alcohol

Vinyl hexanol

RN: 3391-86-4 MP (°C):

MW: 128.22 BP (°C): 174

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.557E-02	1.996E+00	25	D425	0 0 0 0 0	

1615. C₈H₁₆O

Hexyl methyl ketone

2-Octanone

Octan-2-one

RN: 111-13-7**MP (°C):** -16.0**MW:** 128.22**BP (°C):** 172.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.276E-02	4.200E+00	0	C423	0 0 0 0 0	
2.574E-02	3.300E+00	4	C423	0 0 0 0 0	
1.716E-02	2.200E+00	10	C423	0 0 0 0 0	
7.013E-03	8.992E-01	20	D052	1 1 0 0 0	
1.014E-02	1.300E+00	25	C435	0 0 0 0 0	

1616. C₈H₁₆O

Caprylic aldehyde

Octaldehyde

n-Octanal**RN:** 124-13-0**MP (°C):****MW:** 128.22**BP (°C):** 163.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.368E-03	5.600E-01	25	A049	1 0 0 0 1	
1.887E-03	2.420E-01	25	L450	0 0 0 0 0	

1617. C₈H₁₆O₂

Ethyl hexanoate

Ethyl butyl acetate

Ethyl caproate

Ethyl *n*-hexanoate

Ethyl caproate (Nat. C-6 ethyl ester)

RN: 123-66-0**MP (°C):****MW:** 144.22**BP (°C):** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-03	4.500E-01	0	C423	0 0 0 0 0	
3.606E-03	5.200E-01	4	C423	0 0 0 0 0	
3.952E-03	5.700E-01	10	C423	0 0 0 0 0	
4.507E-03	6.500E-01	25	C435	0 0 0 0 0	
4.467E-03	6.442E-01	ns	S460	0 0 0 0 0	

1618. C₈H₁₆O₂

Valproic acid

Vistora

Valporal

Convulex

Depakote

Dalpro

RN: 99-66-1**MP (°C):** 120–130**MW:** 144.22**BP (°C):** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.014E-03	1.300E+00	ns	K444	0 0 0 0 0	
1.380E-02	1.991E+00	ns	S460	0 0 0 0 0	

1619. C₈H₁₆O₂

2-Ethylhexoic acid

2-Ethyl-1-hexanoic acid

3-Heptanecarboxylic acid

Butylethylacetic acid

RN: 149-57-5**MP (°C):****MW:** 144.22**BP (°C):** 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-02	1.498E+00	25	O011	1 0 1 1 1	

1620. C₈H₁₆O₂

3-Hydroxy-2,2,5,5-tetramethyltetrahydrofuran

3-Furanol, 2-ethyltetrahydro-2,2,5,5-tetramethyl-

RN: 29839-74-5**MP (°C):****MW:** 144.22**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.304E-01	9.091E+01	rt	B066	0 2 0 0 1	

1621. C₈H₁₆O₂

n-Butyl n-butylate

Butyl butyrate

RN: 109-21-7**MP (°C):****MW:** 144.22**BP (°C):** 165

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.465E-03	4.998E-01	20	D052	1 1 0 0 0	

1622. C₈H₁₆O₂

Pentyl propionate

Propanoic acid pentyl ester

Amyl *n*-propanoate*n*-Pentyl propionate

RN: 624-54-4

MP (°C):

MW: 144.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	7.067E-01	20	S006	1 0 0 0 1	

1623. C₈H₁₆O₂

3-Hydroxy-2,2-diethyltetrahydrofuran

RN: MP (°C):

MW: 144.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-01	1.961E+01	rt	B066	0 2 0 0 0	

1624. C₈H₁₆O₂*sec*-Hexyl acetate

Methyl amyl acetate

RN: 108-84-9 MP (°C): -64

MW: 144.22 BP (°C): 140

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.543E-03	7.994E-01	20	D052	1 1 0 0 0	

1625. C₈H₁₆O₂

Isobutyl isobutyrate

Isobutyl 2-methylpropanoate

2-Methylpropyl 2-methylpropanoate

IBIB

RN: 97-85-8 MP (°C): -81

MW: 144.22 BP (°C): 147

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.952E-03	5.700E-01	25	A049	1 0 0 0 1	

1626. C₈H₁₆O₂

3-Hydroxy-2-ethyl-5,5-dimethyltetrahydrofuran

3-Furanol, 2-ethyltetrahydro-5,5-dimethyl-

RN: 29839-59-6 **MP (°C):****MW:** 144.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.302E-01	4.762E+01	rt	B066	0 2 0 0 0	

1627. C₈H₁₆O₂

3-Hydroxy-5-ethyl-2,5-dimethyltetrahydrofuran

3-Furanol, 2-ethyltetrahydro-2,5-dimethyl-

RN: 29839-60-9 **MP (°C):****MW:** 144.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E+00	5.000E+02	rt	B066	0 2 0 0 2	

1628. C₈H₁₆O₂

3-Hydroxy-5-methyl-5-propyltetrahydrofuran

3-Furanol, 2-ethyltetrahydro-5-methyl-5-propyl-

RN: 29839-52-9 **MP (°C):****MW:** 144.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-01	1.961E+01	rt	B066	0 2 0 0 0	

1629. C₈H₁₆O₂

Hexyl acetate

2-Ethyl butyl acetate

RN: 142-92-7 **MP (°C):** -80**MW:** 144.22 **BP (°C):** 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.158E-03	5.996E-01	20	D052	1 1 0 0 0	
3.540E-03	5.105E-01	25	M124	2 1 2 2 2	

1630. C₈H₁₆O₂

Caprylic acid

Caprylsäure

RN: 124-07-2

MP (°C): 16.7

MW: 144.22

BP (°C): 239.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.051E-03	4.400E-01	0	B136	1 0 2 1 1	
4.993E-03	7.200E-01	15	F300	1 0 0 0 1	
4.715E-03	6.800E-01	20	B136	1 0 2 1 1	
4.712E-03	6.795E-01	20	D041	1 0 0 0 1	
4.712E-03	6.795E-01	20.0	R001	1 1 1 1 1	
5.478E-03	7.900E-01	30	B136	1 0 2 1 1	
5.471E-03	7.890E-01	30	E005	2 1 1 2 2	
5.474E-03	7.894E-01	30.0	R001	1 1 1 1 1	
5.845E-03	8.430E-01	40	E005	2 1 1 2 2	
6.587E-03	9.500E-01	45	B136	1 0 2 1 1	
6.581E-03	9.491E-01	45.0	R001	1 1 1 1 1	
6.539E-03	9.430E-01	50	E005	2 1 1 2 2	
7.835E-03	1.130E+00	60	B136	1 0 2 1 2	
7.426E-03	1.071E+00	60	E005	2 1 1 2 2	
7.827E-03	1.129E+00	60.0	R001	1 1 1 1 2	
1.803E-02	2.600E+00	100	F300	1 0 0 0 1	
3.050E-03	4.398E-01	.0	R001	1 1 1 1 1	

1631. C₈H₁₆O₃

n-Butyl β-methoxypropionate

Propanoic acid, 3-methoxy-, butyl ester

RN: 4195-88-4 MP (°C):

MW: 160.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.117E-02	9.800E+00	25	R034	0 0 0 0 1	

1632. C₈H₁₆O₃

Amyl lactate

n-Pentyl lactate

RN: 6382-06-5 MP (°C):

MW: 160.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-02	1.000E+01	25	R006	2 2 0 1 2	

1633. C₈H₁₆O₃Methyl β -*n*-butoxypropionate

Butanoic acid, 3-methoxy-3-oxopropyl ester

RN: 40326-33-8 MP (°C):

MW: 160.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.076E-02	8.133E+00	25	R034	0 0 0 0 1	

1634. C₈H₁₆O₃*n*-Propyl β -ethoxypropionate

Propionic acid, 3-ethoxy-, propyl ester

RN: 14144-34-4 MP (°C):

MW: 160.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.466E-02	1.517E+01	25	D002	1 2 1 1 2	

1635. C₈H₁₆O₃

Butylcellosolve acetate

Ethylene glycol monobutyl ether acetate

Ektasolve EB acetate

n-Butyl cellosolve acetateEthylene glycol mono-*n*-butyl ether acetate

RN: 112-07-2 MP (°C):

MW: 160.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.567E-02	8.920E+00	20	D052	1 1 0 0 0	

1636. C₈H₁₆O₃

2,2,5,5-Tetramethyltetrahydrofuran-3,4-diol

3,4-Furandiol, tetrahydro-2,2,5,5-tetramethyl-

RN: 29839-67-6 MP (°C):

MW: 160.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.674E-01	9.091E+01	rt	B066	0 2 0 0 1	

1637. C₈H₁₆O₃S

1,2-Oxathiolane, 5-pentyl-, 2,2-dioxide
 1-Octanesulfonic acid, 3-hydroxy-, γ -sultone
RN: 5633-87-4 **MP (°C):**
MW: 192.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	2.499E-01	20	B058	1 2 0 0 1	
7.938E-02	1.526E+01	100	B058	1 2 0 0 2	

1638. C₈H₁₆O₄

Metaldehyde
 Acetaldehyde homopolymer
 Acetaldehyde tetramer
RN: 9002-91-9 **MP (°C):** 112
MW: 176.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-03	2.000E-01	17	M161	1 0 0 0 2	

1639. C₈H₁₇Cl

1-Chlorooctane
 1-Octylchloride
n-Octyl chloride
 Octyl chloride
RN: 111-85-3 **MP (°C):** -61
MW: 148.68 **BP (°C):** 182

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.270E+01	3.375E+03	5.0	S454	0 0 0 0 0	
2.210E+01	3.286E+03	10.0	S454	0 0 0 0 0	
2.260E+01	3.360E+03	9.9	S454	0 0 0 0 0	
2.350E+01	3.494E+03	9.9	S454	0 0 0 0 0	
2.370E+01	3.524E+03	9.9	S454	0 0 0 0 0	
2.540E+01	3.776E+03	19.1	S454	0 0 0 0 0	
2.470E+01	3.672E+03	25.0	S454	0 0 0 0 0	
2.620E+01	3.895E+03	25.1	S454	0 0 0 0 0	
2.580E+01	3.836E+03	25.2	S454	0 0 0 0 0	
2.710E+01	4.029E+03	30.0	S454	0 0 0 0 0	
2.700E+01	4.014E+03	34.8	S454	0 0 0 0 0	
2.800E+01	4.163E+03	35.1	S454	0 0 0 0 0	
2.690E+01	3.999E+03	35.1	S454	0 0 0 0 0	
2.750E+01	4.089E+03	40.0	S454	0 0 0 0 0	

1640. C₈H₁₇N

D-Conine

 α -Propylpiperidine

D-Coniin

Coniine

RN: 458-88-8

MP (°C): -2

MW: 127.23

BP (°C): 166–167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-01	1.800E+01	19.5	F300	1 0 0 0 1	
7.782E-02	9.901E+00	25	D004	0 0 0 0 0	

1641. C₈H₁₇NO

Ethylbutylacetamide

2-Ethylhexanamide

EBD

RN: 4164-92-5

MP (°C):

MW: 143.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.072E-02	4.400E+00	37	H347	0 0 0 0 0	

1642. C₈H₁₇NO

Ethylisobutylacetamide

2-Ethyl-4-methylpentanamide

EID

RN: 130482-28-9 MP (°C):

MW: 143.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.002E-02	4.300E+00	ns	H348	0 0 0 0 0	

1643. C₈H₁₇NO

Caprylylamide

Caprylsaeure-amid

RN: 629-01-6 MP (°C):

MW: 143.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.288E-02	4.710E+00	100	F300	1 0 0 0 2	

1644. C₈H₁₇NO

Propylisopropylacetamide
 2-Isopropyl-2-propylacetamide
 2-Isopropylvaleramide

PID

RN: 6098-19-7 **MP (°C):**
MW: 143.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.444E-02	3.500E+00	37	H347	0 0 0 0 0	

1645. C₈H₁₇NO

2-Isopropyl-3-methyl-butyramide
 3-Methyl-2-(1-methylethyl)butanamide
 Diisopropylacetamide

RN: 5440-65-3 **MP (°C):**
MW: 143.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.002E-02	4.300E+00	ns	H348	0 0 0 0 0	

1646. C₈H₁₇NO

Dimethylbutylacetamide
 2,2-Dimethylhexanamide
 DBD

RN: 20923-67-5 **MP (°C):**
MW: 143.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.374E-02	3.400E+00	ns	H348	0 0 0 0 0	

1647. C₈H₁₇NO

Valnoctamide
 VCD
 Valmethamide

2-Ethyl-3-methyl-pentanamide
RN: 4171-13-5 **MP (°C):**
MW: 143.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.074E-02	8.700E+00	ns	H348	0 0 0 0 0	

1648. C₈H₁₇NO

Methylpentylacetamide
2-Methyl-heptanamide

MPD

RN: 4164-91-4 **MP (°C):**
MW: 143.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.957E-02	7.100E+00	37	H347	0 0 0 0 0	

1649. C₈H₁₇NO₂

n-Heptyl carbamate
Heptyl carbamate

RN: 4248-20-8 **MP (°C):** 66
MW: 159.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-03	3.822E-01	37	H006	1 2 2 1 1	

1650. C₈H₁₇NO₃

N-Isoamylurethane

RN: **MP (°C):**
MW: 175.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.329E-02	4.082E+00	20	O021	1 0 0 0 0	

1651. C₈H₁₈

2,3,4-Trimethylpentane
2,3,4-Trojmetylopentan

RN: 565-75-3 **MP (°C):** -110
MW: 114.23 **BP (°C):** 113

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.048E-05	2.340E-03	0	P003	2 2 2 2 2	
1.191E-05	1.360E-03	25	K119	1 0 0 0 2	
2.013E-05	2.300E-03	25	P003	2 2 2 2 2	
1.191E-05	1.360E-03	25	P051	2 1 1 2 2	
1.191E-05	1.360E-03	25.00	P007	2 1 2 2 2	

1652. C₈H₁₈

3-Methylheptane

3-Methyloheptan

RN: 589-81-1

MP (°C): -121

MW: 114.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.539E-05	2.900E-03	23	C332	0 0 0 0 0	
6.933E-06	7.920E-04	25	K119	1 0 0 0 2	
6.933E-06	7.920E-04	25	P051	2 1 1 2 2	
6.933E-06	7.920E-04	25.00	P007	2 1 2 2 2	

1653. C₈H₁₈

Isooctane

2:2:4-Trimethylpentane

RN: 540-84-1

MP (°C):

MW: 114.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.153E-05	2.460E-03	0	P003	2 2 2 2 2	
1.226E-05	1.400E-03	20	M337	2 1 2 2 1	
9.980E-06	1.140E-03	25	K119	1 0 0 0 2	
2.136E-05	2.440E-03	25	M001	2 1 2 2 2	
2.136E-05	2.440E-03	25	M002	2 1 2 2 2	
2.136E-05	2.440E-03	25	M130	1 0 0 0 2	
1.795E-05	2.050E-03	25	P003	2 2 2 2 2	
9.980E-06	1.140E-03	25	P051	2 1 1 2 2	
9.980E-06	1.140E-03	25.00	P007	2 1 2 2 2	
7.879E-06	9.000E-04	ns	B170	0 0 0 0 2	
7.500E-05	8.567E-03	ns	J300	0 0 0 0 0	

1654. C₈H₁₈

3,4-Dimethylhexane

RN: 583-48-2

MP (°C):

MW: 114.23

BP (°C): 118

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.998E-06	7.994E-04	ns	S460	0 0 0 0 0	

1655. C₈H₁₈

3-Ethylhexane

Ethyl hexane

RN: 619-99-8

MP (°C):

MW: 114.23

BP (°C): 119

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.076E-06	3.514E-04	ns	S460	0 0 0 0 0	

1656. C₈H₁₈

2,4-Dimethylhexane

RN: 589-43-5

MP (°C):

MW: 114.23

BP (°C): 109

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-05	1.294E-03	ns	S460	0 0 0 0 0	

1657. C₈H₁₈

2,3-Dimethylhexane

2:3-Dimethylhexane

RN: 590-73-8

MP (°C):

MW: 114.23

BP (°C): 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.751E-06	2.000E-04	ns	B170	0 0 0 0 2	

1658. C₈H₁₈

2-Methylheptane

RN: 592-27-8

MP (°C): -109

MW: 114.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.327E-05	3.800E-03	23	C332	0 0 0 0 0	

1659. C₈H₁₈NO₄PS₂

Vamidothion

O,O-Dimethyl *S*-2-(1-*N*-methylcarbamoylethylmercapto)ethyl thiophosphate

RN: 2275-23-2 MP (°C): 35.5

MW: 287.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.392E+01	4.000E+03	20	M161	1 0 0 0 0	
1.392E+01	4.000E+03	ns	M061	0 0 0 0 2	

1660. C₈H₁₈N₂ODi-*n*-butylnitrosamine*N*-Nitroso-di-*n*-butylamine

Dibutylnitrosamine

RN: 924-16-3 MP (°C):

MW: 158.25 BP (°C): 234

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	1.266E+00	24	D083	2 0 0 0 0	
7.574E-03	1.199E+00	rt	I307	0 0 0 0 0	

1661. C₈H₁₈O

2-Octanol

sec-Caprylic alcohol*sec*-Octyl alcohol

Methyl hexyl carbinol

RN: 123-96-6 MP (°C): -38.6

MW: 130.23 BP (°C): 178.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.158E-02	1.508E+00	15	M073	1 0 2 2 2	
8.131E-03	1.059E+00	20	A015	1 2 1 1 2	
8.600E-03	1.120E+00	20	H330	0 0 0 0 0	
3.059E-02	3.984E+00	25	C093	2 1 1 1 0	
9.829E-03	1.280E+00	25	M073	1 0 2 2 2	
7.892E-03	1.028E+00	ns	J300	0 0 0 0 0	

1662. C₈H₁₈O

bis(2-Methyl propyl) ether

iso-Butyl ether

Di-isobutyl ether

RN: 628-55-7 MP (°C):

MW: 130.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.059E+00	1.379E+02	25	M375	2 2 2 1 1	
1.227E-02	1.597E+00	51	M375	2 2 2 1 1	
1.002E+00	1.304E+02	60	M375	2 2 2 1 1	

1663. C₈H₁₈O

DL-2-Octanol

DL-Octanol-(2)

RN: 4128-31-8 MP (°C): -31.6

MW: 130.23 BP (°C): 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.152E-02	1.500E+00	15	F300	1 0 0 0 1	
9.214E-03	1.200E+00	25	F300	1 0 0 0 1	

1664. C₈H₁₈O

2-Ethyl-1-hexanol

Octyl alcohol

Octyl-(2-ethyl hexyl) alcohol

2-Ethyl hexanol

2-Ethylhexanol

2-Ethyhexan-1-ol

RN: 104-76-7 **MP (°C):** -76**MW:** 130.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.012E-02	1.318E+00	10.2	S307	1 1 0 2 2	
9.586E-03	1.248E+00	19.8	S307	1 1 0 2 2	
4.604E-03	5.996E-01	20	D052	1 1 0 0 0	
6.760E-03	8.804E-01	20	H330	0 0 0 0 0	
9.982E-04	1.300E-01	25	K072	1 0 1 1 1	
7.441E-03	9.691E-01	29.6	S307	1 1 0 2 1	
8.437E-03	1.099E+00	40.1	S307	1 1 0 2 2	
5.678E-03	7.395E-01	50.2	S307	1 1 0 2 1	
6.598E-03	8.593E-01	60.3	S307	1 1 0 2 1	
7.594E-03	9.890E-01	70.1	S307	1 1 0 2 1	
8.284E-03	1.079E+00	80.1	S307	1 1 0 2 2	
8.973E-03	1.169E+00	90.3	S307	1 1 0 2 2	

1665. C₈H₁₈O

1-Octanol

Caprylic alcohol

n-Octyl alcohol

n-Octanol

RN: 111-87-5 **MP (°C):** -16**MW:** 130.23 **BP (°C):** 194

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.224E-03	4.198E-01	20	A015	1 2 1 1 2	
3.680E-03	4.793E-01	20	H330	0 0 0 0 0	
3.761E-03	4.898E-01	20.5	S307	1 1 0 2 1	
3.236E-03	4.214E-01	20.96	B178	1 1 0 1 2	EFG
3.162E-03	4.118E-01	23.58	B178	1 1 0 1 2	EFG
2.700E-03	3.516E-01	24	H345	0 0 0 0 0	
4.497E-03	5.857E-01	25	B038	1 2 1 1 2	
3.820E-02	4.975E+00	25	C093	2 1 1 1 0	sic
1.000E+00	1.302E+02	25	F044	1 0 0 0 0	EFG
1.060E-03	1.380E-01	25	J035	0 0 0 0 0	
3.830E-03	4.988E-01	25	J302	2 1 2 2 2	
3.800E-03	4.949E-01	25	K025	2 2 1 1 2	
4.530E-03	5.900E-01	25	K072	1 0 1 1 1	
3.970E-03	5.170E-01	25	L322	1 1 2 2 1	
4.530E-03	5.900E-01	25	M087	1 1 2 1 1	
4.110E-03	5.353E-01	25	S359	2 1 2 2 2	

(continued)

1665. C₈H₁₈O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.671E-03	9.990E-01	30	R067	0 0 0 0 0	
4.911E-03	6.396E-01	30.6	S307	1 1 0 2 1	
3.236E-03	4.214E-01	34.53	B178	1 1 0 1 2	EFG
1.075E-03	1.400E-01	40	J035	0 0 0 0 0	
4.988E-03	6.496E-01	40.1	S307	1 1 0 2 1	
8.054E-03	1.049E+00	50.0	S307	1 1 0 2 2	
3.548E-03	4.621E-01	60	B178	1 1 0 1 2	EFG
6.751E-03	8.792E-01	60.3	S307	1 1 0 2 1	
3.548E-03	4.621E-01	69.31	B178	1 1 0 1 2	EFG
5.908E-03	7.694E-01	70.3	S307	1 1 0 2 1	
6.675E-03	8.692E-01	80.1	S307	1 1 0 2 1	
6.598E-03	8.593E-01	90.3	S307	1 1 0 2 1	
4.514E-03	5.879E-01	ns	L003	0 0 2 1 2	

1666. C₈H₁₈O*n*-Butyl ether

Butyl ether

Dibutyl ether

RN: 142-96-1

MP (°C): -98

MW: 130.23

BP (°C): 142.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.418E-02	1.847E+00	24.80	O005	2 0 2 2 2	
2.700E-03	3.516E-01	25	K012	1 0 0 0 1	
6.138E-03	7.994E-01	25.50	O005	2 0 2 2 0	
1.720E-02	2.240E+00	37	E028	1 0 1 1 2	

1667. C₈H₁₈O₂

Ethohexadiol

2-Ethyl-1,3-hexanediol

RN: 94-96-2

MP (°C): -40

MW: 146.23

BP (°C): 244.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.103E-02	6.000E+00	20	M161	1 0 0 0 0	
2.756E-01	4.031E+01	25	C093	2 1 1 1 1	
2.756E-01	4.031E+01	ns	M061	0 0 0 0 1	

1668. C₈H₁₈O₄S₂

Sulfonethylmethane

Trional

RN: 76-20-0 **MP (°C):** 75
MW: 242.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E-02	4.975E+00	16	A072	1 0 1 0 1	
2.063E-02	5.000E+00	16	F300	1 0 0 0 0	
2.042E-02	4.948E+00	ns	R427	0 0 0 0 0	

1669. C₈H₁₉N

Octylamine

1-Aminooctane

1-Octanamine

Monoctylamine

n-Octylamine

RN: 111-86-4 **MP (°C):** -5
MW: 129.25 **BP (°C):** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.547E-03	2.000E-01	25	K072	1 0 1 1 1	
1.547E-03	2.000E-01	25	M087	1 1 2 1 1	

1670. C₈H₁₉N*n*-DibutylamineDi-*n*-butylamine*N,N*-Dibutylamine*N*-Butyl-1-butanamine

RN: 111-92-2 **MP (°C):** -62
MW: 129.25 **BP (°C):** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-02	3.231E+00	25	K012	1 0 0 0 1	

1671. C₈H₁₉O₂PS₂

Ethoprop

Ethoprophos

O-Ethyl-*S,S*-dipropylphosphorodithioate

Holdem

Rovokil

Ethyl *S,S*-dipropyl phosphorodithioate

RN: 13194-48-4 **MP (°C):**
MW: 242.34 **BP (°C):** 88.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.095E-03	7.500E-01	ns	M161	0 0 0 0 2	
3.097E-03	7.506E-01	ns	S460	0 0 0 0 0	

1672. C₈H₁₉O₂PS₃

Disulfoton

Phosphorodithioic acid *O,O*-diethyl *S*-[2-(ethylthio)ethyl] ester

Solvirex

Disyston

Thiodemeton

Ethylthiometon

RN: 298-04-4 MP (°C): 108

MW: 274.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.940E-05	1.630E-02	19.50	B169	2 1 1 1 2	
9.111E-05	2.500E-02	20	M061	1 0 0 0 1	
5.888E-05	1.616E-02	ns	S460	0 0 0 0 0	
9.111E-05	2.500E-02	rt	M161	0 0 0 0 1	

1673. C₈H₁₉O₃P

Dibutyl hydrogen phosphonate

Di-*n*-butyl phosphite

Dibutoxyphosphine oxide

RN: 1809-19-4 MP (°C):

MW: 194.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.759E-02	7.300E+00	25	B070	1 2 0 1 1	

1674. C₈H₁₉O₃PS₂

Demetonthione

Thiophosphorsaeure-*O,O*-diaethyl-*O*-[2-(ethylthio)-ethyl]-ester*O,O*-Diethyl-*O*-(2-(ethylthio)-ethyl)ester thiophosphoric acid*O,O*-Diethyl 2-ethylmercaptoethyl thiophosphate

Systox

Thiolo-demeton

RN: 298-03-3 MP (°C):

MW: 258.34 BP (°C): 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-04	6.000E-02	20	M061	1 0 0 0 1	
7.742E-03	2.000E+00	rt	M161	0 0 0 0 0	form II
2.323E-04	6.000E-02	rt	M161	0 0 0 0 1	form I
1.277E-02	3.300E+00	rt	M161	0 0 0 0 1	

1675. C₈H₁₉O₃PS₂

Demetonthiol

Thiophosphorsaeure-*O,O*-diaethyl-*S*-[2-(ethylthio)-ethyl]-ester*O,O*-Diethyl-*S*-(2-(ethylthio)-ethyl)ester thiophosphoric acid**RN:** 126-75-0 **MP (°C):****MW:** 258.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.742E-03	2.000E+00	20	F300	1 0 0 0 0	

1676. C₈H₁₉O₄P

Diethyl butyl phosphate

Butyl diethyl phosphate

RN: 2737-00-0 **MP (°C):****MW:** 210.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.136E-02	1.500E+01	25	B070	1 2 0 1 1	

1677. C₈H₁₉O₄P

Diethyl isobutyl phosphate

Ethyl isobutyl phosphate

Phosphoric acid, diethyl 2-methylpropyl ester

RN: 26628-97-7 **MP (°C):****MW:** 210.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.660E-02	1.400E+01	25	B070	1 2 0 1 1	

1678. C₈H₁₉O₄PS₃

Disulfoton sulfone

Phosphorodithioic acid *O,O*-diethyl *S*-[2-(ethylsulfonyl)ethyl] ester

Disulfoton dioxide

Diethyl *S*-(2-ethylsulfonylethyl) phosphorodithioate

Disyston sulfone

Thiodemeton sulfone

RN: 2497-06-5 **MP (°C):****MW:** 306.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.716E-03	8.323E-01	20	B169	2 2 1 1 1	

1679. C₈H₂₀Si

Tetraethylsilicane

Tetraethylsilane

Tetraethylsilicon

RN: 631-36-7 **MP (°C):**
MW: 144.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.250E-06	3.248E-04	25	D346	0 0 0 0 0	

1680. C₈H₂₀Sn

Tetraethyltin

Tetraethylstannane

RN: 597-64-8 **MP (°C):** -112
MW: 234.94 **BP (°C):** 181

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-06	2.678E-04	25	D346	1 1 2 2 2	

1681. C₈H₂₀O₅P₂S₂

Sulfotep

Pirofos

Tetraethyl dithiopyrophosphate

RN: 3689-24-5 **MP (°C):**
MW: 322.32 **BP (°C):** 137.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.307E-05	3.000E-02	20	F300	1 0 0 0 0	
7.756E-05	2.500E-02	20	M061	1 0 0 0 1	
7.756E-05	2.500E-02	rt	M161	0 0 0 0 1	

1682. C₈H₂₃N₅

Tetraethylenepentamine

1,4,7,10,13-Pentaazatridecane

N-(2-Aminoethyl)-N'-(2-((2-aminoethyl)amino)ethyl)-1,2-ethanediamine

1,11-Diamino-3,6,9-triazaundecane

3,6,9-Triaza-1,11-undecanediamine

3,6,9-Triazaundecane-1,11-diamine

RN: 112-57-2 **MP (°C):** -40
MW: 189.31 **BP (°C):** 340

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.582E+00	8.674E+02	4.50	C022	1 2 0 0 2	

1683. C₈Cl₄N₂

Chlorothalonil

2,4,5,6-Tetrachloro-1,3-benzeneddicarbonitrile

Forturf

Exotherm

Bravo

RN: 1897-45-6 MP (°C): 250.5

MW: 265.91 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.256E-06	6.000E-04	25	M161	1 0 0 0 0	

1684. C₉H₄Cl₃NO₂S

Folpet

N-(Trichloromethylthio)phthalimide

Folpan

Folpel

Phaltan

Phalton

RN: 133-07-3 MP (°C): 177

MW: 296.56 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-06	1.005E-03	20	B179	0 0 0 0 0	
3.372E-06	1.000E-03	20	F311	1 2 2 2 1	
3.388E-06	1.005E-03	ns	R427	0 0 0 0 0	

1685. C₉H₅Cl₃N₄

Anilazine

4,6-Dichloro-*N*-(2-chlorophenyl)-1,3,5-triazin-2-amine

Triasyn

Direx

Dyrene

Kemate

RN: 101-05-3 MP (°C): 159.5

MW: 275.53 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.629E-05	1.000E-02	ns	B160	0 0 0 0 1	

1686. C₉H₆ClNO₃S

Benazolin

7-Chloro-2-oxo-3(2H)-benzothiazolacetic acid

Galipan

Herbazolin

Leymin

Metizolin

RN: 3813-05-6 **MP (°C):** 193**MW:** 243.67 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.462E-03	6.000E-01	20	M161	1 0 0 0 2	

1687. C₉H₆Cl₂N₂O₃

Methazole

2-(3,4-Dichlorophenyl)-4-methyl-1,2,4-oxadiazolidine-3,5-dione

Tunic

Paxilon

Chlormethazole

Mezopur

RN: 20354-26-1 **MP (°C):** 123**MW:** 261.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.746E-06	1.500E-03	24	C105	2 1 2 2 2	
5.746E-06	1.500E-03	25	M161	1 0 0 0 1	
5.746E-06	1.500E-03	25	W314	1 0 0 0 1	

1688. C₉H₆Cl₆O₃S

Endosulfan

RN: 115-29-7 **MP (°C):** 209**MW:** 406.93 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.987E-07	3.250E-04	ns	V414	0 0 0 0 0	

1689. C₉H₆Cl₆O₃S α -Endosulfan5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, *endo*-

Endosulfan I

Endosulfan A

Hexachloro-5-norbornene-2,3-dimethanol, cyclic sulfite, *endo*-

Thiodan I

RN: 959-98-8 MP (°C): 109

MW: 406.93 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-06	5.099E-04	20	B300	2 0 1 1 2	
1.302E-06	5.300E-04	25	W025	1 0 2 2 2	
4.030E-07	1.640E-04	ns	A069	0 0 0 0 2	
1.253E-06	5.100E-04	ns	V414	0 0 0 0 0	

1690. C₉H₆Cl₆O₃S β -Endosulfan5-Norbornene-2,3-dimethanol, 1,4,5,6,7,7-hexachloro-, cyclic sulfite, *exo*-

Endosulfan II

Hexachloro-5-norbornene-2,3-dimethanol, cyclic sulfite, *exo*-

Thiodan II

RN: 33213-65-9 MP (°C): 209

MW: 406.93 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.106E-06	4.501E-04	20	B300	2 0 1 1 2	
6.881E-07	2.800E-04	25	W025	1 0 2 2 2	
1.720E-07	7.000E-05	ns	A069	0 0 0 0 1	
1.106E-06	4.500E-04	ns	V414	0 0 0 0 0	

1691. C₉H₆I₃NO₃

2,4,6-Triiodo-3-acetaminobenzoic acid

Acetrizoic acid

RN: 85-36-9 MP (°C):

MW: 556.87 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.299E-03	1.280E+00	25	L025	1 0 0 0 2	
3.232E-03	1.800E+00	50	L025	1 0 0 0 2	
5.387E-03	3.000E+00	100	L025	1 0 0 0 2	
2.442E-03	1.360E+00	ns	H055	0 0 0 0 0	

1692. C₉H₆N₂S

4-Cyanobenzyl isothiocyanate

p-Cyanobenzyl isothiocyanateIsothiocyanic acid, *p*-cyanobenzyl ester**RN:** 3694-48-2 **MP (°C):****MW:** 174.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	5.575E-02	25	D014	1 0 0 0 1	

1693. C₉H₆O₂

Coumarin

Cumarin

1,2-Benzopyrone

2H-1-Benzopyran-2-one

Benzopyran-2-one

Benzopyrone

RN: 91-64-5 **MP (°C):** 70**MW:** 146.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.153E-03	8.992E-01	.2	D073	1 1 2 1 0	
8.211E-03	1.200E+00	0	F300	1 0 0 0 1	
1.298E-02	1.896E+00	20	D073	1 1 2 1 1	
1.368E-02	2.000E+00	22.5	G301	0 0 0 0 0	
1.706E-02	2.494E+00	25	I312	0 0 0 0 0	
1.774E-02	2.593E+00	30	D073	1 1 2 1 1	
1.847E-02	2.700E+00	30	F300	1 0 0 0 1	
3.065E-02	4.480E+00	40	D073	1 1 2 1 1	
4.419E-02	6.458E+00	50	D073	1 1 2 1 1	
4.756E-02	6.951E+00	60	D073	1 1 2 1 1	
1.342E-01	1.961E+01	100	I312	0 0 0 0 0	
1.507E-02	2.203E+00	ns	R082	0 0 0 0 0	
6.842E-04	9.999E-02	rt	D021	0 0 1 1 0	sic

1694. C₉H₆O₃

7-Hydroxycoumarin

Umbelliferone

RN: 93-35-6 **MP (°C):** 230**MW:** 162.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-03	3.110E-01	ns	R082	0 0 0 0 0	

1695. C₉H₆O₅

Phthalonic acid

Phthalonsaeure

RN: 528-46-1

MP (°C):

MW: 194.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.756E+00	5.350E+02	15	F300	1 0 0 0 2	

1696. C₉H₆O₆

Trimesic acid

1,3,5-Benzenetricarboxylic acid

Benzol-tricarbonsaeure-(1,3,5)

RN: 554-95-0

MP (°C):

MW: 210.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.808E-02	3.800E+00	16	F300	1 0 0 0 1	
1.252E-01	2.630E+01	23	F300	1 0 0 0 2	

1697. C₉H₆O₆

1,2,3-Benzenetricarboxylic acid

Benzol-tricarbonsaeure-(1,2,3)

Hemimellitic acid

RN: 569-51-7

MP (°C): 223

MW: 210.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.456E-01	3.060E+01	19	F300	1 0 0 0 2	

1698. C₉H₆O₆

Hydristic acid

Hydrastsaeure

RN: 490-26-6

MP (°C):

MW: 210.14

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.855E-02	6.000E+00	15	F300	1 0 0 0 1	

1699. C₉H₇Cl₃O₃

Trichloroethyl salicylate

Benzoic acid, 2-hydroxy-, 2,2,2-trichloroethyl ester

RN: 56529-85-2 MP (°C):

MW: 269.51 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.081E-03	1.100E+00	37	D009	1 2 1 1 1	0.1N HCl

1700. C₉H₇Cl₃O₃

Silvex

2-(2,4,5-Trichlorophenoxy)propionic acid

Fenoprop

Propionic acid, 2(2,4,5-trichlorophenoxy)-

RN: 93-72-1 MP (°C): 181.6

MW: 269.51 BP (°C): 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-04	7.088E-02	24.99	N417	0 0 0 0 0	
2.634E-04	7.100E-02	25	B164	1 0 1 1 1	
5.195E-04	1.400E-01	25	B185	0 0 0 0 0	
6.678E-04	1.800E-01	25	B200	1 0 0 0 1	
5.195E-04	1.400E-01	25	L024	1 0 0 0 2	
5.194E-04	1.400E-01	25	M061	1 0 0 0 1	
5.195E-04	1.400E-01	25	M161	1 0 0 0 2	
5.194E-04	1.400E-01	ns	B100	0 0 0 0 1	
5.195E-04	1.400E-01	ns	K138	0 0 0 0 1	

1701. C₉H₇N

Quinoline

Chinolin

1-Azanaphthalene

Benzopyridine

1-Benzazine

Benzo[b]pyridine

RN: 91-22-5 MP (°C): -15

MW: 129.16 BP (°C): 237.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.730E-02	6.110E+00	20	A050	0 0 0 0 0	
4.913E-02	6.346E+00	20.3	L339	2 0 2 2 2	
4.968E-02	6.417E+00	40.0	L339	2 0 2 2 2	
6.337E-02	8.185E+00	64.8	L339	2 0 2 2 2	
8.136E-02	1.051E+01	80.2	L339	2 0 2 2 2	
1.063E-01	1.373E+01	100.0	L339	2 0 2 2 2	

1702. C₉H₇NO

4-Hydroxyquinoline

4-Hydroxy-chinolin

4-Quinolinol

RN: 611-36-9 MP (°C): 201

MW: 145.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-02	4.800E+00	15	F300	1 0 0 0 1	

1703. C₉H₇NO

5-Hydroxyquinoline

5-Quinolinol

RN: 578-67-6 MP (°C): 223

MW: 145.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.869E-03	4.165E-01	20	A035	1 0 2 2 1	
2.884E-03	4.187E-01	ns	R427	0 0 0 0 0	

1704. C₉H₇NO

6-Hydroxyquinoline

6-Quinolinol

RN: 580-16-5 MP (°C): 192

MW: 145.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.882E-03	9.990E-01	20	A035	1 0 2 2 1	

1705. C₉H₇NO

7-Hydroxyquinoline

7-Quinolinol

RN: 580-20-1 MP (°C):

MW: 145.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.130E-03	4.543E-01	20	A035	1 0 2 2 1	
3.162E-03	4.590E-01	ns	R427	0 0 0 0 0	

1706. C₉H₇NO

8-Hydroxyquinoline

8-Quinolinol

Hydroxybenzopuridine

RN: 148-24-3**MP (°C):** 76**MW:** 145.16**BP (°C):** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.825E-03	5.552E-01	20	A035	1 0 2 2 1	
4.470E-03	6.489E-01	25.2	P024	2 1 1 1 2	
5.380E-03	7.810E-01	30.3	P024	2 1 1 1 2	

1707. C₉H₇NO

Carbostyryl

2-Hydroxyquinoline

2-Quinolinol

RN: 59-31-4**MP (°C):** 199.0**MW:** 145.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.244E-03	1.052E+00	20	C035	1 0 2 2 1	

1708. C₉H₇NO

3-Hydroxyquinoline

3-Quinolinol

RN: 580-18-7**MP (°C):****MW:** 145.16**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.050E-03	5.879E-01	20	A035	1 0 2 2 1	

1709. C₉H₇NOS

m-Acetylphenyl isothiocyanate

3-Acetylphenyl isothiocyanate

RN: 3125-71-1**MP (°C):****MW:** 177.23**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-05	8.330E-03	25	K032	2 2 0 1 1	

1710. C₉H₇NOS*p*-Acetylphenyl isothiocyanate

4-Acetylphenyl isothiocyanate

RN: 2131-57-9 **MP (°C):****MW:** 177.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-05	1.684E-02	25	D019	1 1 1 1 1	

1711. C₉H₇NOS

Phenacyl thiocyanate

RN: 5399-30-4 **MP (°C):****MW:** 177.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.971E-03	3.494E-01	22	J420	0 0 0 0 0	pH 6.5

1712. C₉H₇NO₂S*m*-Acetoxyphenyl isothiocyanateMethyl *m*-isothiocyanobenzoate**RN:** 3530-01-6 **MP (°C):****MW:** 193.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-04	5.256E-02	25	K032	2 2 0 1 2	
7.700E-04	1.488E-01	25	K032	2 2 0 1 2	

1713. C₉H₇NO₅

2-(Oxaylamo)benzoic acid

Oxanil-carbonsaeure-(2)

Oxanil-*o*-carboxylic acid**RN:** 5651-01-4 **MP (°C):****MW:** 209.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.259E-03	1.100E+00	10	F300	1 0 0 0 1	

1714. C₉H₇N₃S

Tricyclazole

Methyl-1,2,4-triazolo(3,4-b)benzothiazole

5-Methyl-1,2,4-triazolo[3,4-b]benzothiazole

RN: 41814-78-2 **MP (°C):** 187.5**MW:** 189.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.455E-03	1.600E+00	25	M161	1 0 0 0 1	

1715. C₉H₇N₇O₂S

Azathioprine

Cytostatics

Imuran

Azatioprin

6-(1-Methyl-*p*-nitro-5-imidazolyl)-thiopurine

Ccucol

RN: 446-86-6 **MP (°C):** 243.5**MW:** 277.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.689E-04	1.300E-01	24	N016	0 0 0 0 0	
4.472E-04	1.240E-01	25	N063	1 1 1 1 2	intrinsic
4.689E-04	1.300E-01	25	N063	1 1 1 1 2	
3.607E-05	1.000E-02	ns	K444	0 0 0 0 0	

1716. C₉H₈Cl₂O₃

Dichlorprop

Dichloroprop

α-(2,4-Dichlorophenoxy)propionic acid

RN: 120-36-5 **MP (°C):** 117.5**MW:** 235.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.489E-03	3.500E-01	20	L024	1 0 0 0 2	
1.489E-03	3.500E-01	20	M161	1 0 0 0 2	
1.490E-03	3.503E-01	24.99	N417	0 0 0 0 0	
3.527E-03	8.290E-01	25	B164	1 0 1 1 2	
3.020E-03	7.100E-01	28	B200	1 0 0 0 1	
1.484E-02	3.488E+00	ns	B100	0 0 0 0 1	

1717. C₉H₈Cl₂O₃

Methyl (2,4-Dichlorophenoxy)acetate

2,4-Dichlorophenoxyacetic acid methyl ester

RN: 5335-03-5 **MP (°C):****MW:** 235.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.657E-04	1.800E-01	ns	B185	0 0 0 0 0	
5.333E-04	1.254E-01	ns	M120	0 0 1 1 2	

1718. C₉H₈Cl₃NO₂S

Captan

N-Trichloromethylthio-4-cyclohexene-1,2-dicarboximide

Vancide 89

Merpan 90

Orthocid-83

Pillarcap

RN: 133-06-2 MP (°C): 178

MW: 300.59 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-06	4.989E-04	20	B179	0 0 0 0 0	
<1.66E-06	<5.00E-04	20	F311	1 2 2 2 1	
1.544E-05	4.642E-03	ns	H322	0 0 0 0 0	
1.660E-06	4.989E-04	ns	R427	0 0 0 0 0	
1.663E-06	5.000E-04	rt	M161	0 0 0 0 0	

1719. C₉H₈N₂OS

m-Acetamidophenyl isothiocyanate

3-Acetamidophenyl isothiocyanate

RN: 3137-83-5 MP (°C):

MW: 192.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.950E-04	5.671E-02	25	K032	2 2 0 1 2	

1720. C₉H₈N₄O₆

Nifurtoinol

3-(Hydroxymethyl)nitrofurantoin

RN: 1088-92-2 MP (°C):

MW: 268.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-03	3.300E-01	22	B154	1 1 1 1 1	0.1M HCl

1721. C₉H₈O

(E)-Cinnamaldehyde

(E)-3-Phenylpropenal;

(2E)-3-Phenyl-2-propenal

(E)-3-Phenylprop-2-enone

(E)-3-Phenylacrolein

(E)-3-Phenylprop-2-enal

RN: 14371-10-9 MP (°C):

MW: 132.16 BP (°C): 250–253

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-02	1.850E+00	25	D407	1 0 2 2 2	

1722. C₉H₈O

Cinnamaldehyde

3-Phenyl-2-propenal

Phenylacrolein

3-Phenyl-2-propenaldehyde

Zimtaldehyde

RN: 104-55-2**MP (°C):****MW:** 132.16**BP (°C):** 246

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	1.348E+00	25	I019	1 0 1 2 2	
9.100E-03	1.203E+00	37	E028	1 0 1 1 1	

1723. C₉H₈O₂*trans*-Cinnamic acid*trans*-3-Phenyl-2-propenoic acid*trans*-β-Phenylacrylic acid

(E)-3-Phenyl-2-propenoic acid

RN: 140-10-3 **MP (°C):** 133**MW:** 148.16 **BP (°C):** 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.417E-03	2.100E-01	15	M461	0 0 0 0 0	
2.700E-03	4.000E-01	18	F300	1 0 0 0 0	
2.835E-03	4.200E-01	18	M077	1 2 1 1 2	
3.010E-03	4.460E-01	25	C090	1 2 2 2 2	
3.685E-03	5.460E-01	25	M077	1 2 1 1 2	
1.552E-03	2.300E-01	25	M461	0 0 0 0 0	
2.092E-03	3.100E-01	30	M461	0 0 0 0 0	
5.264E-03	7.800E-01	35	M077	1 2 1 1 2	
4.252E-03	6.300E-01	40	M461	0 0 0 0 0	
7.364E-03	1.091E+00	45	M077	1 2 1 1 2	
5.737E-03	8.500E-01	50	M461	0 0 0 0 0	

1724. C₉H₈O₂

Atropic acid

Atropasaeure

RN: 492-38-6 **MP (°C):** 106**MW:** 148.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.774E-03	1.300E+00	20	F300	1 0 0 0 1	

1725. C₉H₈O₂

Cinnamic acid

Phenylacrylic acid

3-Phenylpropenoic acid

2-Propenoic acid, 3-phenyl-

RN: 621-82-9 **MP (°C):** 133
MW: 148.16 **BP (°C):** 261.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.024E-03	2.999E-01	10	M043	1 0 0 0 0	
3.390E-03	5.023E-01	14.3	D061	1 0 0 0 2	
2.642E-03	3.914E-01	16.3	D061	1 0 0 0 2	
2.643E-03	3.916E-01	16.30	B118	1 0 0 0 2	unit assumed
1.515E-02	2.245E+00	20	C092	2 1 0 1 1	sic
2.699E-03	3.998E-01	20	M043	1 0 0 0 0	
3.170E-03	4.697E-01	22	E045	2 0 1 1 2	
3.260E-03	4.830E-01	23	E045	2 0 1 1 2	
3.360E-03	4.978E-01	24	E045	2 0 1 1 2	
3.450E-03	5.112E-01	25	E045	2 0 1 1 2	
3.850E-03	5.704E-01	25	K040	1 0 2 1 2	
3.340E-03	4.949E-01	25	L048	1 2 2 1 2	
3.340E-03	4.949E-01	25	L050	2 0 1 2 2	
3.540E-03	5.245E-01	26	E045	2 0 1 1 2	
3.800E-03	5.630E-01	26.4	P043	2 0 1 1 2	
3.630E-03	5.378E-01	27	E045	2 0 1 1 2	
4.963E-03	7.353E-01	28	D050	1 2 1 2 2	
4.688E-03	6.946E-01	30	B118	1 0 0 0 2	unit assumed
4.682E-03	6.937E-01	30	D061	1 0 0 0 2	
4.047E-03	5.996E-01	30	M043	1 0 0 0 0	
3.959E-02	5.865E+00	100	M043	1 0 0 0 1	

1726. C₉H₈O₂

cis-Cinnamic acid

cis-Zimtsaeure

RN: 102-94-3 **MP (°C):**
MW: 148.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.657E-02	6.900E+00	18	F300	1 0 0 0 1	
4.644E-02	6.880E+00	18	M077	1 2 1 1 2	form III, mp 68 C
5.143E-02	7.620E+00	18	M077	1 2 1 1 2	form II, mp 58 C
6.041E-02	8.950E+00	18	M077	1 2 1 1 2	form I, mp 42 C
5.703E-02	8.450E+00	25	M077	1 2 1 1 2	form III, mp 68 C
6.324E-02	9.370E+00	25	M077	1 2 1 1 2	form II, mp 58 C
7.445E-02	1.103E+01	25	M077	1 2 1 1 2	form I, mp 42 C
7.519E-02	1.114E+01	35	M077	1 2 1 1 2	form III, mp 68 C
8.362E-02	1.239E+01	35	M077	1 2 1 1 2	form II, mp 58 C

(continued)

1726. C₉H₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.861E-02	1.461E+01	35	M077	1 2 1 1 2	form I, mp 42 C
9.760E-02	1.446E+01	45	M077	1 2 1 1 2	form III, mp 68 C
1.086E-01	1.609E+01	45	M077	1 2 1 1 2	form II, mp 58 C
1.245E-01	1.845E+01	55	M077	1 2 1 1 2	form III, mp 68 C

1727. C₉H₈O₃

2-Acetophenone carboxylic acid

Acetophenon-carbonsaeure-(2)

o-Carboxyacetophenone

RN: 577-56-0 MP (°C):
 MW: 164.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-02	3.984E+00	rt	H431	0 0 0 0 0	

1728. C₉H₈O₄

Homophthalic acid

Homophthalsaeure

RN: 89-51-0 MP (°C): 184.5
 MW: 180.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E-02	4.579E+00	rt	H431	0 0 0 0 0	

1729. C₉H₈O₄

Caffeic acid

3,4-Dihydroxy-*trans*-cinnamate

(E)-3-(3,4-Dihydroxyphenyl)-2-propenoic acid

RN: 331-39-5 MP (°C): 196 C
 MW: 180.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.053E-03	5.500E-01	15	M461	0 0 0 0 0	
5.440E-03	9.800E-01	25	M461	0 0 0 0 0	
6.827E-03	1.230E+00	30	M461	0 0 0 0 0	
1.132E-02	2.040E+00	40	M461	0 0 0 0 0	
1.621E-02	2.920E+00	50	M461	0 0 0 0 0	

1730. C₉H₈O₄

4-Methylphthalic acid

RN: 4316-23-8

MP (°C): 149

MW: 180.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.211E-02	3.984E+00	rt	H431	0 0 0 0 0	

1731. C₉H₈O₄

Aspirin

Acetyl-salicylsaeure

Acetylsalicylic acid

RN: 50-78-2

MP (°C): 135

MW: 180.16

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-02	5.623E+00	4.62	M053	1 0 1 1 0	EFG, 0.1N HCl
1.107E-02	1.995E+00	12.55	M053	1 0 1 1 0	EFG, 0.1N HCl
3.200E-02	5.765E+00	14	O019	1 0 0 1 2	
1.998E-02	3.600E+00	15	E017	1 0 0 0 0	EFG
1.388E-02	2.500E+00	15	F300	1 0 0 0 1	
1.716E-02	3.091E+00	15	H022	1 2 2 2 2	
2.109E-02	3.800E+00	20	E017	1 0 0 0 0	EFG
1.460E-02	2.630E+00	20.96	M053	1 0 1 1 0	EFG, 0.1N HCl
1.769E-02	3.188E+00	22.5	B422	2 0 2 2 2	
2.553E-02	4.600E+00	25	E017	1 0 0 0 0	EFG
2.775E-02	5.000E+00	25	S304	1 2 1 2 2	form IV
2.131E-02	3.840E+00	25	S304	1 2 1 2 2	form I
2.442E-02	4.400E+00	25	S304	1 2 1 2 2	form II
1.890E-02	3.405E+00	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.62, intrinsic
2.500E-02	4.504E+00	30	A065	2 0 2 2 1	
2.831E-02	5.100E+00	30	E017	1 0 0 0 0	EFG
2.387E-02	4.300E+00	30	G042	1 1 1 1 1	0.1N HCl
2.851E-02	5.137E+00	30	H022	1 2 2 2 2	
2.000E-02	3.603E+00	30	L069	1 0 1 1 0	EFG
2.637E-02	4.750E+00	30	S304	1 2 1 2 2	form I
3.275E-02	5.900E+00	30	S304	1 2 1 2 2	form IV
3.108E-02	5.600E+00	30	S304	1 2 1 2 2	form II
3.275E-02	5.900E+00	35	E017	1 0 0 0 0	EFG
2.942E-02	5.300E+00	37	D009	1 2 1 1 1	0.1N HCl
3.219E-02	5.800E+00	37	G042	1 1 1 1 1	0.1N HCl
3.641E-02	6.560E+00	37	G430	0 0 0 0 0	pH 4.5
3.569E-02	6.430E+00	37	K086	1 0 0 0 2	
3.031E-02	5.460E+00	37	M115	2 2 1 1 2	
4.052E-02	7.300E+00	37	S304	1 2 1 2 2	form II
3.830E-02	6.900E+00	37	S304	1 2 1 2 2	form I
4.218E-02	7.600E+00	37	S304	1 2 1 2 2	form IV
3.441E-02	6.200E+00	37	Y421	0 0 0 0 0	

(continued)

1731. C₉H₈O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.830E-02	6.900E+00	40	E017	1 0 0 0 0	EFG
4.385E-02	7.900E+00	40	S304	1 2 1 2 2	form II
4.218E-02	7.600E+00	40	S304	1 2 1 2 2	form I
4.607E-02	8.300E+00	40	S304	1 2 1 2 2	form IV
4.662E-02	8.400E+00	45	E017	1 0 0 0 0	EFG
4.274E-02	7.700E+00	45	G042	1 1 1 1 1	0.1N HCl
5.551E-02	1.000E+01	49.42	M053	1 0 1 1 0	EFG, 0.1N HCl
4.940E-02	8.900E+00	50	G042	1 1 1 1 1	0.1N HCl
6.829E-02	1.230E+01	60.17	M053	1 0 1 1 0	EFG, 0.1N HCl
1.848E-02	3.330E+00	ns	K444	0 0 0 0 0	
1.551E-02	2.795E+00	rt	R431	0 0 0 0 0	Average

1732. C₉H₉ClO₃

DL-2-(2-Chlorophenoxy)propionic acid

2-(*o*-Chlorophenoxy)propionic acid

3-CP

RN: 76466-16-5 MP (°C): 113

MW: 200.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.974E-03	1.199E+00	22	B200	1 0 0 0 1	
9.726E-02	1.951E+01	100	B200	1 0 0 0 2	

1733. C₉H₉ClO₃

DL-2-(4-Chlorophenoxy)propionic acid

RN: 3307-39-9 MP (°C):

MW: 200.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.352E-03	1.475E+00	25	B164	1 0 1 1 2	
7.352E-03	1.475E+00	25	B185	0 0 0 0 0	

1734. C₉H₉ClO₃

(4-Chloro-2-methylphenoxy)acetic acid

MCPA

RN: 94-74-6 MP (°C): 120.0

MW: 200.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.138E-03	6.296E-01	20	M061	1 0 0 0 1	
5.852E-03	1.174E+00	25	B164	1 0 1 1 2	
5.852E-03	1.174E+00	25	B185	0 0 0 0 0	
7.975E-03	1.600E+00	25	B185	0 0 0 0 0	

(continued)

1734. C₉H₉ClO₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.979E-03	9.990E-01	ns	B100	0 0 0 0 0	
3.190E-03	6.400E-01	ns	B185	0 0 0 0 0	
4.112E-03	8.250E-01	ns	L024	0 0 0 0 2	
4.112E-03	8.250E-01	rt	M161	0 0 0 0 2	

1735. C₉H₉Cl₂NO

Propanil

3',4'-Dichloropropionanilide

DPA

RN: 709-98-8 MP (°C): 85
 MW: 218.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.961E-04	1.300E-01	20	F311	1 2 2 2 1	
2.293E-03	5.000E-01	ns	B185	0 0 0 0 0	
2.292E-03	4.998E-01	ns	B200	0 0 0 0 0	
2.293E-03	5.000E-01	ns	H042	0 0 0 0 2	
1.032E-03	2.250E-01	rt	M161	0 0 0 0 2	

1736. C₉H₉Cl₂NO₂

Dichlormate

3,4-Dichlorobenzyl N-methylcarbamate

Romate

RN: 1966-58-1 MP (°C): 52
 MW: 234.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.262E-04	1.700E-01	25	B200	1 0 0 0 2	

1737. C₉H₉Cl₂NO₂

UC 22463

Sirmate 4E

Rowmate

Sirmate

RN: 62046-37-1 MP (°C): 52
 MW: 234.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.262E-04	1.700E-01	ns	H042	0 0 0 0 2	

1738. C₉H₉I₂NO₃

L-3,5-Diiodotyrosine

3,5-Diido-L-tyrosine

DIT

RN: 300-39-0 MP (°C): 213

MW: 432.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-03	6.196E-01	25	D041	1 0 0 0 1	

1739. C₉H₉I₂NO₃

3,5-Diiodotyrosine

3,5-Diiod-DL-tyrosin

DL-Thyronin

RN: 66-02-4 MP (°C): 204

MW: 432.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-03	4.500E-01	15	F300	1 0 0 0 1	
7.850E-04	3.399E-01	25	D041	1 0 0 0 1	
1.386E-03	6.000E-01	25	F300	1 0 0 0 0	
1.316E-02	5.700E+00	75	F300	1 0 0 0 1	

1740. C₉H₉N

Skatole

3-Methyl-indol

3-Methylindole

RN: 83-34-1 MP (°C): 95

MW: 131.18 BP (°C): 265.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.430E-03	4.500E-01	16	F300	1 0 0 0 0	

1741. C₉H₉NOS

m-Ethoxyphenyl isothiocyanate

3-Ethoxyphenyl isothiocyanate

RN: 3701-44-8 MP (°C):

MW: 179.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-04	6.811E-02	25	K032	2 2 0 1 2	

1742. C₉H₉NOS*p*-Ethoxyphenyl isothiocyanate

4-Ethoxyphenyl isothiocyanate

RN: 25687-50-7 MP (°C):

MW: 179.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-05	9.858E-03	25	D019	1 1 1 1 1	

1743. C₉H₉NO₂*p*-AcetamidobenzaldehydeAcetamide, *N*-(4-formylphenyl)-

Acetanilide, 4'-formyl-

Micotiazone

RN: 122-85-0 MP (°C):

MW: 163.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-02	3.247E+00	25	D044	0 0 0 0 0	

1744. C₉H₉NO₃

Hippuric acid

Hippursaeure

N-Benzoylglycine

Benzoylaminoacetic acid

RN: 495-69-2 MP (°C): 187

MW: 179.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E-02	3.289E+00	20	D041	1 0 0 0 1	
2.177E-02	3.900E+00	20	F300	1 0 0 0 1	
2.050E-02	3.673E+00	25	B028	1 0 0 0 2	
2.048E-02	3.670E+00	25	K053	2 2 2 2 2	
2.095E-02	3.754E+00	25	L048	1 2 2 1 2	
2.095E-02	3.754E+00	25	L050	2 0 1 2 2	
2.048E-02	3.670E+00	25.1	N026	0 0 0 0 0	
3.320E-02	5.949E+00	38	B028	1 0 0 0 2	
2.334E-02	4.182E+00	rt	D021	0 0 1 1 1	

1745. C₉H₉NO₃

Acetamide, 2-(benzoyloxy)-
Glycolamide, benzoate

RN: 64649-43-0 **MP (°C):** 121
MW: 179.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.288E-02	4.100E+00	22	B427	1 0 0 1 1	in 0.01M HCl
2.288E-02	4.100E+00	22	N317	1 1 2 1 2	

1746. C₉H₉NO₄

Benzadox
((Benzoylamino)oxy)acetic acid

Topicide
RN: 5251-93-4 **MP (°C):**
MW: 195.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.069E-02	1.575E+01	ns	B100	0 0 0 0 1	

1747. C₉H₉NS

p-Methylbenzyl isothiocyanate
4-Methylbenzyl isothiocyanate
RN: 3694-46-0 **MP (°C):**
MW: 163.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	2.612E-02	25	D014	1 0 0 0 1	

1748. C₉H₉N₃OS

Benzthiazuron
Benzothiazol-2-yl-3-methylurea
N-2-Benzothiazoly-N'-methylurea
Gatnon

RN: 1929-88-0 **MP (°C):**
MW: 207.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.790E-05	1.200E-02	20	M161	1 0 0 0 1	

1749. C₉H₉N₃O₂

Carbendazim

1H-Benzimidazol-2-ylcarbamic acid methyl ester

RN: 10605-21-7 MP (°C): 302

MW: 191.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.034E-05	5.800E-03	20	A064	1 0 1 1 1	
3.034E-05	5.800E-03	20	M161	1 0 0 0 1	pH 7

1750. C₉H₉N₃O₂S₂

Sulfathiazole

Sulphathiazole

N1-2-Thiazolyl-

4-Amino-N-2-thiazolyl-

RN: 72-14-0 MP (°C): 202

MW: 255.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-03	3.600E-01	16	H114	1 0 0 0 1	
1.743E-03	4.450E-01	20	F073	1 2 2 2 2	
1.958E-03	5.000E-01	20	F074	1 0 0 0 2	
4.426E-03	1.130E+00	20	K028	2 1 2 1 2	pH 7.3, form I
1.414E-03	3.610E-01	20	K028	2 1 2 1 2	pH 3.8, form II
2.460E-03	6.280E-01	20	K028	2 1 2 1 2	pH 7.3, form II
2.483E-03	6.340E-01	20	K028	2 1 2 1 2	pH 3.8, form I
1.347E-03	3.439E-01	20	L058	1 0 1 1 1	
2.482E-03	6.336E-01	20	M042	1 0 0 0 2	pH 3.8, form I, mp 200-202 C
1.413E-03	3.609E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 175 C
1.305E-03	3.332E-01	25	F415	0 0 0 0 0	Average
1.461E-03	3.730E-01	25	H005	1 0 1 2 2	average of 4
1.821E-03	4.650E-01	25	K096	1 2 2 2 2	α form
3.290E-03	8.400E-01	25	K096	1 2 2 2 2	β form
1.796E-03	4.586E-01	25	M440	0 0 0 0 0	
1.966E-03	5.020E-01	26	C102	2 0 2 2 2	
2.350E-03	6.000E-01	26	L052	1 0 0 0 0	
2.270E-03	5.796E-01	30	H018	0 0 0 0 0	
4.308E-03	1.100E+00	30	K096	1 2 2 2 2	β form
2.327E-03	5.940E-01	30	K096	1 2 2 2 2	α form
2.544E-03	6.496E-01	30	M046	1 0 0 0 1	
4.460E-03	1.139E+00	30.0	H010	2 2 1 1 2	
3.564E-03	9.100E-01	35	H114	1 0 0 0 1	
3.094E-03	7.900E-01	35	K096	1 2 2 2 2	α form
5.354E-03	1.367E+00	35	K096	1 2 2 2 2	β form
3.760E-03	9.600E-01	37	C102	2 0 2 2 2	
3.564E-03	9.100E-01	37	D084	1 0 1 0 1	
3.678E-03	9.391E-01	37	F072	1 0 0 0 2	

(continued)

1750. C₉H₉N₃O₂S₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.686E-03	9.411E-01	37	F075	1 0 2 2 2	
3.443E-03	8.790E-01	37	K091	1 0 0 0 2	
2.560E-03	6.536E-01	37	K095	2 0 0 0 2	intrinsic
3.838E-03	9.800E-01	37	L091	1 0 0 0 1	pH 5.5
3.721E-03	9.500E-01	37	M057	1 0 0 0 2	pH 5.5
3.799E-03	9.700E-01	37	R044	0 0 0 0 0	
3.756E-03	9.591E-01	37.50	M142	1 0 0 0 1	
3.603E-03	9.200E-01	38	K006	1 0 0 0 2	
6.619E-03	1.690E+00	40	K096	1 2 2 2 2	β form
4.073E-03	1.040E+00	40	K096	1 2 2 2 2	α form
8.284E-03	2.115E+00	45	K096	1 2 2 2 2	β form
5.288E-03	1.350E+00	45	K096	1 2 2 2 2	α form
6.592E-03	1.683E+00	49	K096	1 2 2 2 2	α form
9.964E-03	2.544E+00	49	K096	1 2 2 2 2	β form
1.683E-03	4.298E-01	ns	L044	0 0 0 0 2	
3.467E-03	8.853E-01	ns	R427	0 0 0 0 0	
1.918E-03	4.898E-01	rt	N015	0 0 2 2 2	

1751. C₉H₁₀

Indan

2,3-Dihydroindene

Hydrindane

1H-Indene, 2,3-dihydro-

Hydrindane

RN: 496-11-7

MP (°C): -51.4

MW: 118.18

BP (°C): 176.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.232E-04	1.091E-01	25	M064	1 1 2 2 2	
7.522E-04	8.890E-02	25	P051	2 1 1 2 2	
9.232E-04	1.091E-01	ns	M344	0 0 0 0 2	

1752. C₉H₁₀

α-Methylstyrene

2-Phenyl-1-propene

Isopropenylbenzene

2-Phenylpropene

β-Phenylpropene

RN: 98-83-9

MP (°C): -24.0

MW: 118.18

BP (°C): 167.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-04	1.155E-01	ns	D001	0 0 0 0 2	

1753. C₉H₁₀BrClN₂O₂

Chlorbromuron

3-(4-Bromo-3-chlorophenyl)-1-methoxy-1-methylurea

N'-(4-Bromo-3-chlorophenyl)-N-methoxy-N-methylurea

Maloran

RN: 13360-45-7 MP (°C):

MW: 293.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-04	3.529E-02	20	B179	0 0 0 0 0	
1.192E-04	3.500E-02	20	M161	1 0 0 0 1	
1.703E-04	5.000E-02	ns	B200	0 0 0 0 1	
1.703E-04	5.000E-02	ns	G036	0 0 0 0 1	

1754. C₉H₁₀Cl₂N₂O

Diuron

1,1-Dimethyl-3-(3,4-dichlorophenyl)urea

3-(3,4-Dichlorophenyl)-1,1-dimethylurea

RN: 330-54-1 MP (°C): 158

MW: 233.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-04	4.242E-02	20	B179	0 0 0 0 0	
9.438E-05	2.200E-02	20	E048	1 2 1 1 1	
1.716E-04	4.000E-02	25	A039	1 1 0 0 2	
1.802E-04	4.200E-02	25	B185	0 0 0 0 0	
1.802E-04	4.200E-02	25	B200	1 0 0 0 1	
1.802E-04	4.200E-02	25	G036	1 0 0 0 1	
1.802E-04	4.200E-02	25	G099	1 0 0 1 0	
1.600E-04	3.730E-02	25	H073	2 1 1 2 2	
1.802E-04	4.200E-02	25	M061	1 0 0 0 1	
1.802E-04	4.200E-02	25	M161	1 0 0 0 1	
1.802E-04	4.200E-02	25	N333	0 0 0 0 0	
1.716E-04	4.000E-02	ns	B160	0 0 0 0 1	
1.802E-04	4.200E-02	ns	H042	0 0 0 0 1	
1.000E+02	2.331E+04	ns	H342	0 0 0 0 0	EFG, <i>sic</i>
1.802E-04	4.200E-02	ns	K007	0 0 0 0 1	
1.995E-04	4.651E-02	ns	M163	0 0 0 0 0	EFG
1.802E-04	4.200E-02	ns	V414	0 0 0 0 0	

1755. C₉H₁₀Cl₂N₂O₂

Linuron

3-(3,4-Dichlorophenyl)-1-methoxy-1-methylurea

RN: 330-55-2 MP (°C): 93

MW: 249.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-04	7.523E-02	20	B179	0 0 0 0 0	
3.011E-04	7.500E-02	25	B185	0 0 0 0 0	

(continued)

1755. C₉H₁₀Cl₂N₂O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.011E-04	7.500E-02	25	B200	1 0 0 0 1	
3.011E-04	7.500E-02	25	M061	1 0 0 0 1	
3.011E-04	7.500E-02	25	M161	1 0 0 0 1	
3.252E-04	8.100E-02	25	M162	1 1 0 0 1	
3.011E-04	7.500E-02	ns	K007	0 0 0 0 1	

1756. C₉H₁₀Cl₂O

2,4-Dichloro-6-propyl-phenol

RN: 91399-12-1 **MP (°C):****MW:** 205.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-04	1.005E-01	25	B316	0 0 0 0 0	

1757. C₉H₁₀Cl₃O₃PS

Trichlormetafos-3

O-Methyl O-ethyl O-2,4,5-trichlorophenyl thiophosphate

RN: 2633-54-7 **MP (°C):****MW:** 335.58 **BP (°C):** 127

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.19E-04	<4.00E-02	ns	M061	0 0 0 0 0	

1758. C₉H₁₀NO₃

2-Oxo-5-indolinyl acetate

5-Acetoxy-2-oxindole

RN: 74973-14-1 **MP (°C):****MW:** 180.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-02	5.225E+00	25	A066	1 0 1 1 1	

1759. C₉H₁₀NO₃PS

Cyanophos

Dimethyl O-(*p*-cyanophenyl) phosphorothioate

Ciafos

CYAP

RN: 2636-26-2 **MP (°C):** 14.5**MW:** 243.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.891E-04	4.600E-02	30	M161	1 0 0 0 1	

1760. C₉H₁₀N₂O₂

Phenacemide

Phenylacetyl urea

RN: 63-98-9

MP (°C): 215

MW: 178.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.021E-03	1.820E-01	ns	B404	0 2 1 1 0	

1761. C₉H₁₀N₂O₃*p*-Nitroacetotoluide

4-Nitroacetotoluide

RN: MP (°C):

MW: 194.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.200E+00	rt	F043	0 0 2 1 1	

1762. C₉H₁₀N₂O₃*p*-Ureidophenyl acetate

4-Ureidophenyl acetate

RN: 59746-11-1 MP (°C):

MW: 194.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-03	6.214E-01	25	A066	1 0 1 1 1	

1763. C₉H₁₀N₂O₃*o*-Nitroacetotoluide

2-Nitroacetotoluide

RN: 612-45-3 MP (°C):

MW: 194.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.200E+00	rt	F043	0 0 2 1 1	

1764. C₉H₁₀N₂O₃S₂

Ethoxzolamide

6-Ethoxy-2-benzothiazolesulfonamide

Diuretic C

Cardrase

RN: 452-35-7

MP (°C): 188

MW: 258.32

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.033E-02	25	C415	1 0 0 1 0	
1.548E-04	4.000E-02	ns	M032	0 0 0 0 0	
1.549E-04	4.001E-02	ns	R428	0 0 0 0 0	

1765. C₉H₁₀N₂S

4-Dimethylaminophenyl isothiocyanate

4-Isothiocyanato-*N,N*-dimethyl-benzenamine

RN: 2131-64-8 MP (°C):

MW: 178.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.500E-05	1.337E-02	25	D019	1 1 1 1 1	

1766. C₉H₁₀N₂S

3-Dimethylaminophenyl isothiocyanate

N',N'-Dimethyl-*m*-aminophenyl isothiocyanate

RN: 2392-67-8 MP (°C):

MW: 178.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-04	7.487E-02	25	D019	1 1 1 1 2	
1.950E-04	3.476E-02	25	K032	2 2 0 1 2	

1767. C₉H₁₀N₄

2,6,7-Trimethylpteridine

2:6:7-Trimethylpteridine

RN: 23767-00-2 MP (°C):

MW: 174.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.087E-02	1.235E+01	20	A083	1 2 0 0 0	

1768. C₉H₁₀N₄O₂S₂

Sulfamethizole

Sulfamethylthiadiazole

RN: 144-82-1

MP (°C): 208

MW: 270.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.957E-03	5.290E-01	20	F073	1 2 2 2 2	
3.320E-03	8.975E-01	37	A046	2 0 1 1 2	
3.884E-03	1.050E+00	37	B046	1 0 2 2 2	pH 4.5
3.270E-03	8.840E-01	37	K091	1 0 0 0 2	
3.270E-03	8.840E-01	37	W016	2 0 1 1 2	
2.938E-03	7.943E-01	ns	N057	1 0 2 2 0	EFG, intrinsic

1769. C₉H₁₀O

Propiophenone

1-Phenyl-1-propanone

Ethyl phenyl ketone

Propiophenoë

RN: 93-55-0

MP (°C): 19

MW: 134.18

BP (°C): 217

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.479E-02	1.985E+00	ns	S460	0 0 0 0 0	

1770. C₉H₁₀O₂

Hydrocinnamic acid

Hydrozimtsaeure

RN: 501-52-0

MP (°C): 48

MW: 150.18

BP (°C): 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.929E-02	5.900E+00	20	F300	1 0 0 0 2	
6.162E-02	9.254E+00	30	D033	2 2 1 2 2	
7.668E-02	1.152E+01	40	D033	2 2 1 2 2	

1771. C₉H₁₀O₂

2,5-Dimethylbenzoic acid

2-Carboxy-1,4-dimethylbenzene

Isoxylic acid

RN: 610-72-0

MP (°C): 132.5–134.5

MW: 150.18

BP (°C): 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.199E-03	1.800E-01	25	H007	0 0 0 0 0	

1772. C₉H₁₀O₂

2,4-Dimethylbenzoic acid

4-Carboxy-1,3-dimethylbenzene

RN: 611-01-8 **MP (°C):** 124–126
MW: 150.18 **BP (°C):** 267

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.065E-03	1.600E-01	25	H007	0 0 0 0 0	

1773. C₉H₁₀O₂

Benzyl acetate

Phenylmethyl acetate

Acetic acid phenylmethyl ester

α-Acetoxytoluene

RN: 140-11-4 **MP (°C):** –51.3
MW: 150.18 **BP (°C):** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.973E-03	1.498E+00	25	M350	1 0 1 1 1	

1774. C₉H₁₀O₂

3,4-Dimethylbenzoic acid

1-Carboxy-3,4-dimethylbenzene

RN: 619-04-5 **MP (°C):** 165
MW: 150.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.600E-04	1.292E-01	ns	C014	0 0 0 1 1	

1775. C₉H₁₀O₂

Ethyl benzoate

Ethyl *p*-benzoate

Benzoesaeure-aethyl ester

RN: 93-89-0 **MP (°C):** –34
MW: 150.18 **BP (°C):** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.990E-03	1.200E+00	22	N317	1 1 2 1 2	
4.794E-03	7.200E-01	25	A003	1 2 1 2 1	
6.659E-03	1.000E+00	60	F300	1 0 0 0 0	

1776. C₉H₁₀O₃

4-Hydroxy-3-ethoxybenzaldehyde

Ethylprotal; ethylvanillin

Bourbonal

Ethovan

NSC 67240

Ethavan

RN: 121-32-4 MP (°C): 65

MW: 166.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.019E+00	1.693E+02	25	D407	1 0 2 2 2	

1777. C₉H₁₀O₃

Ethyl salicylate

Ethyl *o*-hydroxybenzoate

RN: 118-61-6 MP (°C): 1-3

MW: 166.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.032E-02	6.700E+00	37	D009	1 2 1 1 1	0.1N HCl

1778. C₉H₁₀O₃

Ethylparaben

4-Hydroxybenzoic acid ethyl ester

Ethyl *p*-hydroxybenzoate

Ethyl 4-hydroxybenzoate

RN: 120-47-8 MP (°C): 116

MW: 166.18 BP (°C): 297

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.750E-03	4.570E-01	15	B355	0 0 0 0 0	
3.370E-03	5.600E-01	20	B355	0 0 0 0 0	
4.910E-03	8.159E-01	20	C006	1 2 1 1 2	
5.329E-03	8.855E-01	25	A059	1 0 1 1 1	
4.090E-03	6.797E-01	25	B355	0 0 0 0 0	
4.510E-03	7.494E-01	25	D081	1 2 2 1 2	
5.300E-03	8.807E-01	25	D339	0 0 0 0 0	
6.310E-03	1.049E+00	25	F322	2 0 1 1 0	EFG
9.628E-03	1.600E+00	25	O027	1 0 1 0 1	
6.379E-03	1.060E+00	25	P013	0 0 0 0 0	
9.500E-03	1.579E+00	27	B129	2 2 2 2 1	
5.200E-03	8.641E-01	27	G078	2 1 0 1 0	EFG
5.400E-03	8.974E-01	27.0	G067	2 0 1 1 1	
6.770E-03	1.125E+00	30	A059	1 0 1 1 2	
8.266E-03	1.374E+00	35	A059	1 0 1 1 2	
7.568E-03	1.258E+00	39.3	G302	2 2 2 2 0	EFG
9.540E-03	1.585E+00	40	A059	1 0 1 1 2	

1779. C₉H₁₀O₃

Methyl-4-methoxybenzoate

Methyl anisate

RN: 121-98-2 **MP (°C):** 49
MW: 166.18 **BP (°C):** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.870E-03	6.431E-01	20	C006	1 0 1 1 2	

1780. C₉H₁₀O₃

DL-Tropic acid

DL-Tropasaeure

RN: 529-64-6 **MP (°C):** 118.5
MW: 166.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.173E-01	1.950E+01	20	F300	1 0 0 0 2	

1781. C₉H₁₀O₄

3,4-Methoxybenzoic acid

Veratrumsaeure

RN: 93-07-2 **MP (°C):**
MW: 182.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-03	5.000E-01	14	F300	1 0 0 0 0	
3.293E-02	6.000E+00	100	F300	1 0 0 0 0	

1782. C₉H₁₁BrN₂O₂

Metobromuron

3-(*p*-Bromophenyl)-1-methoxy-1-methylurea

Patoran

N'-(4-Bromophenyl)-N-methoxy-N-methylurea

Pattonex

RN: 3060-89-7 **MP (°C):**
MW: 259.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.288E-03	3.338E-01	20	B179	0 0 0 0 0	
1.274E-03	3.300E-01	20	B200	1 0 0 0 2	
1.274E-03	3.300E-01	20	G036	1 0 0 0 2	
1.274E-03	3.300E-01	20	M061	1 0 0 0 1	
1.274E-03	3.300E-01	20	M161	1 0 0 0 2	
1.157E-03	2.999E-01	ns	B100	0 0 0 0 0	

1783. C₉H₁₁ClN₂O

Monuron

N'-(4-Chlorophenyl)-N,N-dimethyl-urea

1,1-Dimethyl-3-(*p*-chlorophenyl)urea

RN: 150-68-5 MP (°C): 170.5

MW: 198.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.007E-03	2.000E-01	18	F035	1 0 0 0 0	
1.175E-03	2.334E-01	20	B179	0 0 0 0 0	
1.007E-03	2.000E-01	20	E048	1 2 1 1 2	
1.007E-03	2.000E-01	20	F311	1 2 2 2 1	
1.158E-03	2.300E-01	25	A039	1 1 0 0 2	
1.158E-03	2.300E-01	25	B185	0 0 0 0 0	
1.158E-03	2.300E-01	25	B200	1 0 0 0 2	
1.158E-03	2.300E-01	25	G036	1 0 0 0 2	
1.158E-03	2.300E-01	25	G099	1 0 0 1 0	
1.319E-03	2.620E-01	25	H073	2 1 1 2 2	
1.158E-03	2.300E-01	25	M061	1 0 0 0 2	
1.158E-03	2.300E-01	25	M161	1 0 0 0 2	
1.007E-03	2.000E-01	ns	B100	0 0 0 0 0	
1.158E-03	2.300E-01	ns	B160	0 0 0 0 2	
9.000E-04	1.788E-01	ns	F184	0 0 0 0 0	
1.158E-03	2.300E-01	ns	H112	0 0 0 0 2	
1.158E-03	2.300E-01	ns	K007	0 0 0 0 2	
1.158E-03	2.300E-01	ns	N013	0 0 0 0 2	

1784. C₉H₁₁ClN₂O₂

Monolinuron

3-(4-Chlorophenyl)-1-methoxy-1-methylurea

Arresin

Afesin

Aresin

RN: 1746-81-2 MP (°C): 80

MW: 214.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.692E-03	5.777E-01	20	B179	0 0 0 0 0	
4.333E-03	9.300E-01	20	G036	1 0 0 0 2	
2.702E-03	5.800E-01	20	M061	1 0 0 0 2	
2.702E-03	5.800E-01	22.5	G301	0 0 0 0 0	
3.424E-03	7.350E-01	25	M162	1 1 0 0 2	
2.794E-03	5.996E-01	ns	B100	0 0 0 0 0	
2.702E-03	5.800E-01	rt	M161	0 0 0 0 2	

1785. C₉H₁₁ClO

3-Methyl-5-ethyl-4-chloro-phenol

m-Cresol, 4-chloro-5-ethyl-

RN: 1125-66-2 **MP (°C):**
MW: 170.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	3.754E-01	25	B316	0 0 0 0 0	

1786. C₉H₁₁Cl₂N₃O₄S₂

Methylchlothiazide

2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3-(chloromethyl)-3,4-dihydro-2-methyl-1,1-dioxide

6-Chloro-3-(chloromethyl)-3,4-dihydro-2-methyl-2H-1,2,4-benzothiadiazine-7-sulfonamide 1,1-dioxide

RN: 135-07-9 **MP (°C):**
MW: 360.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.388E-04	5.000E-02	rt	A095	0 0 2 2 0	

1787. C₉H₁₁Cl₃NO₃PS

Chlorpyrifos

O,O-Diethyl *O*-3,5,6-trichloro-2-pyridyl phosphorothioate

DOWCO 179

RN: 2921-88-2 **MP (°C):** 41.5
MW: 350.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.284E-06	4.502E-04	10	B324	0 0 0 0 0	
1.284E-06	4.500E-04	10	B324	0 0 0 0 0	
1.997E-06	7.000E-04	19	B169	2 1 1 1 1	
2.082E-06	7.299E-04	20	B300	2 1 1 1 2	
2.082E-06	7.299E-04	20	B324	0 0 0 0 0	
2.082E-06	7.300E-04	20	B324	0 0 0 0 0	
1.141E-06	4.000E-04	23	B096	1 2 0 0 0	
3.195E-06	1.120E-03	24	F179	2 2 2 2 2	
1.141E-06	4.000E-04	24	K069	2 0 0 1 1	
3.708E-06	1.300E-03	30	B324	0 0 0 0 0	
3.708E-06	1.300E-03	30	B324	0 0 0 0 0	
5.705E-06	2.000E-03	35	M161	1 0 0 0 0	
1.141E-06	4.000E-04	ns	F071	0 1 2 1 0	
8.557E-07	3.000E-04	ns	K138	0 0 0 0 1	
5.705E-06	2.000E-03	ns	M110	0 0 0 0 0	EFG
3.195E-06	1.120E-03	ns	V414	0 0 0 0 0	
5.705E-06	2.000E-03	ns	Y414	0 0 0 0 0	

1788. C₉H₁₁Cl₃NO₄P

Chlorpyrifos oxon

Chlorpyrifos oxygen analog

Dursban oxygen analog

DOWCO 180

3,5,6-Trichloro-2-pyridyl diethyl phosphate

RN: 5598-15-2 **MP (°C):****MW:** 334.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.554E-03	5.200E-01	24	K069	2 0 0 1 1	

1789. C₉H₁₁FN₂O₃

2,4(1H,3H)-Pyrimidinedione, 5-fluoro-3-(1-oxopentyl)-

RN: 145303-99-7 **MP (°C):****MW:** 214.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	1.071 E+00	22	B416	2 2 1 2 1	

1790. C₉H₁₁FN₂O₄

1-Butyryloxymethyl-5-fluorouracil

Butanoic acid, (5-fluoro-3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)methyl ester

RN: 66542-37-8 **MP (°C):****MW:** 230.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.170E-02	9.600E+00	22	B321	0 0 0 0 0	pH 4.0
4.170E-02	9.600E+00	22	B332	1 1 0 0 1	pH 4.0
4.952E-02	1.140E+01	22	M317	1 1 1 1 1	

1791. C₉H₁₁FN₂O₄

1-Isobutyloxycarbonyl-5-fluorouracil

1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, 2-methylpropyl ester

RN: 71759-45-0 **MP (°C):****MW:** 230.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-02	3.000E+00	22	B332	1 1 0 0 1	pH 4.0

1792. C₉H₁₁FN₂O₄

1-Butyloxycarbonyl-5-fluorouracil

5-Fluoro-1-(butoxycarbonyl)uracil

RN: 85326-32-5 **MP (°C):****MW:** 230.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.563E-02	5.900E+00	22	B332	1 1 0 0 1	pH 4.0

1793. C₉H₁₁IN₂O₅

2'-Deoxy-5-iodouridine

Idoxuridine

(+) -5-Iodo-2'-deoxyuridine

Herplex

RN: 54-42-2 **MP (°C):** 165**MW:** 354.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.650E+03	2.001E+06	25	N332	0 0 0 0 0	pH 7.4

1794. C₉H₁₁N

1,2,3,4-Tetrahydroquinoline

Kusol

THQ

RN: 635-46-1 **MP (°C):** 15–17**MW:** 133.19 **BP (°C):** 249

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-02	1.404E+00	20.3	L339	2 0 2 2 2	
1.386E-02	1.847E+00	40.0	L339	2 0 2 2 2	
1.774E-02	2.362E+00	59.8	L339	2 0 2 2 2	
2.326E-02	3.098E+00	79.6	L339	2 0 2 2 2	
2.988E-02	3.980E+00	100.4	L339	2 0 2 2 2	

1795. C₉H₁₁NO

N-Methylacetanilide

Acetamide, N-methyl-N-phenyl-

RN: 579-10-2 **MP (°C):** 102**MW:** 149.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-01	2.200E+01	20	B101	0 0 0 0 0	
1.673E-01	2.496E+01	25	B101	0 0 0 0 0	
1.908E-01	2.847E+01	30	B101	0 0 0 0 0	
2.166E-01	3.232E+01	35	B101	0 0 0 0 0	
1.122E-01	1.674E+01	ns	R424	0 0 0 0 0	

1796. C₉H₁₁NO*p*-Aminopropiophenone

4'-Aminopropiophenone

RN: 70-69-9 **MP (°C):** 140
MW: 149.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-03	3.521E-01	37.5	G002	1 1 1 1 2	pH 6.8

1797. C₉H₁₁NO

Propionanilide

Propionsaeure-anilid

Propanilide

RN: 620-71-3 **MP (°C):** 106
MW: 149.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.206E-02	1.800E+00	18	F300	1 0 0 0 1	
1.204E-02	1.797E+00	20	B101	0 0 0 0 0	

1798. C₉H₁₁NO

Methyl, [3-(acetylamino)phenyl]-

m-Toluidin-N-acetat*m*-Toluidine-N-acetate

RN: 113321-22-5 **MP (°C):**
MW: 149.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.949E-02	4.400E+00	13	F300	1 0 0 0 1	

1799. C₉H₁₁NO₂

Phe

(S)-(-)-Phenylalanine

(S)-Phenylalanine

2-Amino-3-phenylpropanoic acid

Phenylalanine

RN: 63-91-2 **MP (°C):** 283
MW: 165.19 **BP (°C):** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.047E-02	9.989E+00	0	D018	2 2 2 1 2	
1.174E-01	1.940E+01	0	F300	1 0 0 0 2	
1.740E-01	2.874E+01	15	D349	2 1 1 2 2	
1.515E-01	2.502E+01	20	B032	1 2 2 1 2	
1.770E-01	2.924E+01	20	D349	2 1 1 2 2	

(continued)

1799. C₉H₁₁NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.637E-01	2.705E+01	25	B032	1 2 2 1 2	
1.740E-01	2.875E+01	25	D041	1 0 0 0 2	
1.800E-01	2.973E+01	25	D349	2 1 1 2 2	
1.816E-01	3.000E+01	25	F300	1 0 0 0 1	
1.649E-01	2.724E+01	25	G092	2 1 1 1 1	
1.649E-01	2.724E+01	25	G315	0 0 0 0 0	
1.625E-01	2.684E+01	25	G433	0 0 0 0 0	
1.589E-01	2.625E+01	25	K031	2 1 2 1 2	
1.200E-01	1.982E+01	25	M097	2 2 2 2 2	
1.494E-01	2.468E+01	25	M374	1 0 2 1 2	
2.100E-01	3.469E+01	25	N001	0 0 0 0 0	EFG
1.720E-01	2.841E+01	25	N012	2 0 2 1 2	
1.574E-01	2.601E+01	25	O316	1 0 1 2 2	
1.575E-01	2.601E+01	25	O316	1 0 1 2 2	
1.689E-01	2.790E+01	25.1	N024	0 0 0 0 0	
1.689E-01	2.790E+01	25.1	N025	0 0 0 0 0	
1.689E-01	2.790E+01	25.1	N026	0 0 0 0 0	
1.649E-01	2.724E+01	25.1	N027	1 1 2 2 2	
1.717E-01	2.837E+01	27	D036	0 0 0 0 0	
1.683E-01	2.780E+01	27	D036	0 0 0 0 0	
1.834E-01	3.030E+01	28	L081	2 1 2 2 2	
1.790E-01	2.957E+01	29.80	B032	1 2 2 1 2	
2.567E-01	4.240E+01	50	F300	1 0 0 0 2	
3.761E-01	6.212E+01	75	D041	1 0 0 0 2	
3.759E-01	6.210E+01	75	F300	1 0 0 0 2	
4.619E-01	7.630E+01	98	M160	2 1 1 1 0	
5.454E-01	9.010E+01	100	F300	1 0 0 0 2	
9.064E-02	1.497E+01	rt	H431	0 0 0 0 0	

1800. C₉H₁₁NO₂

4-(Dimethylamino)benzoic acid

4-Dimethylaminobenzoic acid

RN: 619-84-1 MP (°C): 242.5

MW: 165.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	6.608E-02	ns	C014	0 0 0 1 1	

1801. C₉H₁₁NO₂*p*-Methoxyacetanilide*p*-Acetanisidine*N*-(4-Methoxyphenyl)acetamide*N*-(4-Methoxyphenyl)acetic acid amide*p*-AcetanisidineAcetamide, *N*-(4-methoxyphenyl)-**RN:** 51-66-1 **MP (°C):** 400.3**MW:** 165.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.029E-02	1.700E+00	15	F300	1 0 0 0 1	
8.820E-03	1.457E+00	15	M352	1 1 1 1 2	
7.090E-02	1.171E+01	25	D044	0 0 0 0 0	
1.353E-02	2.234E+00	25	M352	1 1 1 1 2	
2.131E-02	3.521E+00	40	M352	1 1 1 1 2	
3.249E-02	5.367E+00	50	M352	1 1 1 1 2	

1802. C₉H₁₁NO₂

2-Methyl-4-acetaminophenol

3-Methyl-4-hydroxyacetanilide

3-Methylparacetamol

RN: 16375-90-9 **MP (°C):****MW:** 165.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-02	4.189E+00	25	D078	1 2 1 1 2	

1803. C₉H₁₁NO₂

DL-Phenylalanine

DL-Phenylalanin

RN: 150-30-1 **MP (°C):** 166.5**MW:** 165.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.993E-02	9.900E+00	0	F300	1 0 0 0 1	
9.080E-02	1.500E+01	21	F300	1 0 0 0 1	
9.008E-02	1.488E+01	21	P045	1 0 2 1 2	
8.464E-02	1.398E+01	25	D018	2 2 2 1 2	
8.476E-02	1.400E+01	25	D041	1 0 0 0 2	
1.304E-01	2.154E+01	50	D018	2 2 2 1 2	
1.295E-01	2.140E+01	50	F300	1 0 0 0 2	
2.158E-01	3.564E+01	75	D018	2 2 2 1 2	
2.164E-01	3.575E+01	75	D041	1 0 0 0 2	
2.167E-01	3.580E+01	75	F300	1 0 0 0 2	
3.898E-01	6.440E+01	100	F300	1 0 0 0 2	

1804. C₉H₁₁NO₂*m*-Tolyl methylcarbamate

3-Tolyl methylcarbamate

RN: 1129-41-5 **MP (°C):** 76.5
MW: 165.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.574E-02	2.600E+00	30	M161	1 0 0 0 1	

1805. C₉H₁₁NO₂

D-Phenylalanine

D- α -Aminohydrocinnamic acidD- α -Amino- β -phenylpropionic acidD- β -Phenyl- α -aminopropionic acid

D-PHE

RN: 673-06-3 **MP (°C):** 273
MW: 165.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.763E-01	2.913E+01	25	D041	1 0 0 0 0	

1806. C₉H₁₁NO₂Ethyl *p*-aminobenzoate

4-Aminobenzoic acid ethyl ester

Ethyl *p*-aminobenzoic acid

Benzocaine

RN: 94-09-7 **MP (°C):** 89.0
MW: 165.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.308E-03	7.117E-01	15	M352	1 1 1 1 2	
1.513E-02	2.500E+00	20	F300	1 0 0 0 1	
5.800E-03	9.581E-01	25	A418	0 0 0 0 0	
4.840E-03	7.995E-01	25	H008	0 0 0 0 0	
6.493E-03	1.073E+00	25	M352	1 1 1 1 2	
6.216E-03	1.027E+00	25	P303	0 0 0 0 0	
6.980E-03	1.153E+00	30	A418	0 0 0 0 0	
7.930E-03	1.310E+00	30	B071	1 2 1 1 2	
5.150E-03	8.507E-01	30	H018	0 0 0 0 0	
7.500E-03	1.239E+00	30	J018	1 2 0 1 1	0.05N NaOH
7.000E-03	1.156E+00	30	L069	1 0 1 1 0	EFG
7.680E-03	1.269E+00	30	R003	0 0 0 0 0	
8.156E-03	1.347E+00	33	P303	0 0 0 0 0	
8.750E-03	1.445E+00	35	A418	0 0 0 0 0	
1.020E-02	1.685E+00	37	F006	1 1 2 2 2	
1.024E-02	1.692E+00	40	A418	0 0 0 0 0	
1.164E-02	1.924E+00	40	M352	1 1 1 1 2	

(continued)

1806. C₉H₁₁NO₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-02	1.704E+00	40	P303	0 0 0 0 0	
1.701E-02	2.810E+00	50	M352	1 1 1 1 2	
>3.03E-03	>5.00E-01	ns	B404	0 2 1 1 0	
4.810E-03	7.946E-01	ns	M066	0 0 0 0 2	
4.810E-03	7.946E-01	rt	B016	0 0 1 1 2	pH 7.4
5.135E-03	8.483E-01	rt	I404	0 0 0 0 0	Average

1807. C₉H₁₁NO₃

L-Tyrosine

3-(4-Hydroxyphenyl)-L-alanine

Tyrosine

(S)-(-)-Tyrosine

p-Tyrosine

L-Tyrosin

RN: 60-18-4

MP (°C): 342dec

MW: 181.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.241E-03	2.249E-01	0	D018	2 2 2 1 2	
1.104E-03	2.000E-01	0	F300	1 0 0 0 0	
2.042E-03	3.700E-01	20	B032	1 2 2 1 2	
2.495E-03	4.520E-01	21	P045	1 0 2 1 2	
2.285E-03	4.140E-01	22	A045	2 0 2 2 2	
2.800E-03	5.073E-01	24.99	C404	2 1 2 2 1	
7.800E-02	1.413E+01	25	C405	2 1 2 2 2	
2.642E-03	4.788E-01	25	D018	2 2 2 1 2	
2.482E-03	4.498E-01	25	D041	1 0 0 0 1	
2.759E-03	5.000E-01	25	F300	1 0 0 0 0	
2.444E-03	4.428E-01	25	G433	0 0 0 0 0	
2.620E-03	4.747E-01	25	H097	2 2 2 2 2	
2.622E-03	4.750E-01	25.1	N024	0 0 0 0 0	
2.495E-03	4.520E-01	25.1	N025	0 0 0 0 0	
2.489E-03	4.510E-01	25.1	N026	0 0 0 0 0	
2.488E-03	4.508E-01	25.1	N027	1 1 2 2 2	
2.753E-03	4.988E-01	27	D036	0 0 0 0 0	
2.677E-03	4.850E-01	27	D036	0 0 0 0 0	
3.195E-03	5.790E-01	28	L081	2 1 2 2 2	
3.800E-03	6.885E-01	34.99	C404	2 1 2 2 1	
5.050E-03	9.150E-01	44.99	C404	2 1 2 2 1	
6.064E-03	1.099E+00	50	D018	2 2 2 1 2	
6.071E-03	1.100E+00	50	F300	1 0 0 0 1	
1.309E-02	2.372E+00	75	D018	2 2 2 1 2	
1.343E-02	2.434E+00	75	D041	1 0 0 0 2	
1.325E-02	2.400E+00	75	F300	1 0 0 0 1	
3.091E-02	5.600E+00	100	F300	1 0 0 0 1	

1808. C₉H₁₁NO₃

D-Tyrosine

3-(4-Hydroxyphenyl)-D-alanine

RN: 556-02-5 MP (°C): >300

MW: 181.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.482E-03	4.498E-01	25	D041	1 0 0 0 1	
5.789E-03	1.049E+00	50	D041	1 0 0 0 2	

1809. C₉H₁₁NO₃

DL-Tyrosine

DL-Tyrosin

3-(4-Hydroxyphenyl)-DL-alanine

DL-2-Amino-3-(4-hydroxyphenyl)-propanoic acid

RN: 556-03-6 MP (°C): 325

MW: 181.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.519E-04	1.000E-01	0	F300	1 0 0 0 0	
2.208E-03	4.000E-01	20	F300	1 0 0 0 0	
1.936E-03	3.509E-01	25	D041	1 0 0 0 2	
4.610E-03	8.353E-01	50	D041	1 0 0 0 2	
4.415E-03	8.000E-01	50	F300	1 0 0 0 0	
3.753E-02	6.800E+00	100	F300	1 0 0 0 1	

1810. C₉H₁₁NO₄

Dopa

DL-3-(3,4-Dihydroxyphenyl)alanine

DL-Dopa

RN: 63-84-3 MP (°C): >270

MW: 197.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.523E-02	4.975E+00	20	D041	1 0 0 0 0	
1.237E-01	2.439E+01	100	D041	1 0 0 0 1	

1811. C₉H₁₁NO₄

Levodopa

L-3,4-Dihydroxyphenylalanine

RN: 59-92-7 MP (°C): 277

MW: 197.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-02	5.000E+00	20	F300	1 0 0 0 0	
1.917E-02	3.780E+00	25	H015	1 0 0 0 2	

(continued)

1811. C₉H₁₁NO₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.927E-02	3.800E+00	25.1	N025	0 0 0 0 0	
1.268E-01	2.500E+01	100	F300	1 0 0 0 1	
5.071E-03	1.000E+00	ns	K444	0 0 0 0 0	

1812. C₉H₁₁NS₂Hg

Phenylmercury dimethyldithiocarbamate

Chipman merbam

Merfenl 51

Phelam DP

RN: 32407-99-1 MP (°C): 175

MW: 397.91 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.508E-05	6.000E-03	20	M161	1 0 0 0 0	

1813. C₉H₁₁N₃O

Biacetyl mono(2-pyridyl)-hydrazone

BPH

Biacetyl mono(2-pyridyl)hydrazone

RN: 74158-10-4 MP (°C): 95

MW: 177.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.643E-04	9.999E-02	ns	R080	0 0 0 0 0	

1814. C₉H₁₁N₃O₂S₂

Sulfathiazoline

Benzenesulfonamide, 4-amino-N-(4,5-dihydro-2-thiazolyl)-

RN: 32365-02-9 MP (°C):

MW: 257.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.790E-04	1.490E-01	20	F073	1 2 2 2 2	

1815. C₉H₁₁N₃O₄

Orotic acid morpholine

RN: MP (°C): 289–291

MW: 225.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-01	9.909E+01	-4	N018	0 0 0 0 0	
6.500E-01	1.464E+02	16	N018	0 0 0 0 0	
7.450E-01	1.678E+02	25	N018	0 0 0 0 0	

1816. C₉H₁₁O₄P

2-Carboxyethylphenylphosphinic acid
CEPPA

RN: **MP (°C):**
MW: 214.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-02	2.076E+01	25.1	W412	0 0 0 0 0	
1.947E-01	4.171E+01	35.51	W412	0 0 0 0 0	
3.450E-01	7.389E+01	44.92	W412	0 0 0 0 0	
6.388E-01	1.368E+02	54.02	W412	0 0 0 0 0	
1.068E+00	2.287E+02	64.60	W412	0 0 0 0 0	
1.341E+00	2.873E+02	69.60	W412	0 0 0 0 0	
1.536E+00	3.290E+02	71.91	W412	0 0 0 0 0	
1.883E+00	4.034E+02	76.32	W412	0 0 0 0 0	

1817. C₉H₁₂

1,2,3-Trimethylbenzene

Hemimellitene

Hemellitol

RN: 526-73-8 **MP (°C):** -25
MW: 120.20 **BP (°C):** 175

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.450E-04	6.551E-02	25	M342	1 0 1 1 2	
6.256E-04	7.520E-02	25	S005	2 2 2 2 2	
6.256E-04	7.520E-02	25	S191	1 2 2 2 2	
6.256E-04	7.520E-02	25	S358	2 2 2 2 2	

1818. C₉H₁₂

1-Ethyl-2-methylbenzene

2-Ethyltoluene

o-Ethyltoluene

1-Methyl-2-ethylbenzene

RN: 611-14-3 **MP (°C):** -80.8
MW: 120.20 **BP (°C):** 165.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.210E-04	7.464E-02	25	M342	1 0 1 1 2	
7.742E-04	9.305E-02	ns	H123	0 0 0 0 0	

1819. C₉H₁₂

1,8-Nonadiyne

RN: 2396-65-8 **MP (°C):** -21
MW: 120.20 **BP (°C):** 55

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-03	1.250E-01	25	M001	2 1 2 2 2	

1820. C₉H₁₂

Cumene

Isopropylbenzene

Cumol

2-Phenylpropane

RN: 98-82-8

MP (°C): -96

MW: 120.20

BP (°C): 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.694E-04	8.046E-02	24.94	G034	1 2 2 2 2	
6.073E-04	7.300E-02	25	A002	1 2 1 1 1	
4.018E-04	4.830E-02	25	K119	1 0 0 0 2	
4.160E-04	5.000E-02	25	M001	2 1 2 2 2	
4.409E-04	5.300E-02	25	M002	2 2 1 2 1	
4.160E-04	5.000E-02	25	M130	1 0 0 0 1	
4.018E-04	4.830E-02	25	P051	2 1 1 2 2	
5.433E-04	6.530E-02	25	S005	2 2 2 2 2	
5.433E-04	6.530E-02	25	S191	1 2 2 2 2	
5.433E-04	6.530E-02	25	S358	2 1 2 2 2	
4.018E-04	4.830E-02	25.00	P007	2 1 2 2 2	
6.897E-04	8.290E-02	29.94	G034	1 2 2 2 2	
7.124E-04	8.563E-02	34.94	G034	1 2 2 2 2	
7.469E-04	8.978E-02	39.94	G034	1 2 2 2 2	
7.867E-04	9.456E-02	44.94	G034	1 2 2 2 2	
8.353E-04	1.004E-01	49.94	G034	1 2 2 2 2	
8.894E-04	1.069E-01	54.94	G034	1 2 2 2 2	
9.566E-04	1.150E-01	59.94	G034	1 2 2 2 2	
1.035E-03	1.243E-01	65.14	G034	1 2 2 2 2	
1.128E-03	1.355E-01	70.34	G034	1 2 2 2 2	
1.226E-03	1.473E-01	75.04	G034	1 2 2 2 2	
1.345E-03	1.617E-01	80.24	G034	1 2 2 2 2	
4.160E-04	5.000E-02	ns	H123	0 0 0 0 0	
4.160E-04	5.000E-02	ns	M344	0 0 0 0 1	

1821. C₉H₁₂

n-Propylbenzene

1-Phenylpropane

Propylbenzene

Isocomene

RN: 103-65-1

MP (°C): -99.2

MW: 120.20

BP (°C): 159.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-04	5.373E-02	10	O312	2 2 0 2 2	
5.000E-04	6.010E-02	15	F001	1 0 1 2 0	
4.350E-04	5.229E-02	15	O312	2 2 0 2 2	
4.520E-04	5.433E-02	20	O312	2 2 0 2 2	
4.576E-04	5.500E-02	25	A002	1 2 1 1 1	
1.000E-03	1.202E-01	25	K001	1 0 2 1 2	

(continued)

1821. C₉H₁₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.340E-04	5.217E-02	25	M342	1 0 1 1 2	
4.430E-04	5.325E-02	25	O312	2 2 0 2 2	
8.319E-04	9.999E-02	25	S012	2 0 2 2 1	
4.150E-04	4.988E-02	25	S359	2 1 2 2 2	
3.920E-04	4.712E-02	25	T067	2 1 2 1 2	
4.340E-04	5.217E-02	25	W300	2 2 2 2 2	
4.370E-04	5.253E-02	30	O312	2 2 0 2 2	
4.710E-04	5.661E-02	35	O312	2 2 0 2 2	
5.320E-04	6.394E-02	40	O312	2 2 0 2 2	
5.540E-04	6.659E-02	45	O312	2 2 0 2 2	
1.098E-03	1.320E-01	85.8	G035	1 0 0 0 2	
1.381E-03	1.660E-01	114.5	G035	1 0 0 0 2	
2.670E-03	3.209E-01	140.5	G035	1 0 0 0 2	
7.232E-03	8.692E-01	188.0	G035	1 0 0 0 1	
2.033E-02	2.444E+00	222.0	G035	1 0 0 0 2	
4.576E-04	5.500E-02	ns	H123	0 0 0 0 0	
2.700E-02	3.245E+00	ns	H307	0 0 0 0 0	
4.576E-04	5.500E-02	ns	M344	0 0 0 0 1	

1822. C₉H₁₂

1,2,4-Trimethylbenzene

Pseudocumene

RN: 95-63-6 MP (°C): -44
 MW: 120.20 BP (°C): 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.318E-04	5.190E-02	25	K119	1 0 0 0 2	
4.742E-04	5.700E-02	25	M001	2 1 2 2 2	
4.318E-04	5.190E-02	25	P051	2 1 1 2 2	
4.909E-04	5.900E-02	25	S005	2 2 2 2 2	
4.909E-04	5.900E-02	25	S191	1 2 2 2 2	
4.909E-04	5.900E-02	25	S358	2 1 2 2 2	
4.318E-04	5.190E-02	25.00	P007	2 1 2 2 2	
4.742E-04	5.700E-02	ns	M344	0 0 0 0 1	

1823. C₉H₁₂

p-Ethyltoluene

4-Ethyltoluene

1-Ethyl-4-methylbenzene

RN: 622-96-8 MP (°C): -62
 MW: 120.20 BP (°C): 162

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.891E-04	9.485E-02	ns	H123	0 0 0 0 0	

1824. C₉H₁₂

Mesitylene

1,3,5-Trimethylbenzene

Mesitelene

RN: 108-67-8**MP (°C):** -44.8**MW:** 120.20**BP (°C):** 164.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.794E-04	4.560E-02	15	S203	1 1 2 1 2	
3.111E-04	3.740E-02	20	M337	2 1 2 2 2	
8.070E-04	9.700E-02	25	A002	1 2 1 1 1	
4.010E-04	4.820E-02	25	S005	2 2 2 2 2	
4.010E-04	4.820E-02	25	S191	1 2 2 2 2	
4.118E-04	4.950E-02	25	S203	1 1 2 1 2	
4.010E-04	4.820E-02	25	S358	2 1 2 2 2	
3.280E-04	3.942E-02	25.04	V013	2 2 2 2 2	
5.322E-04	6.397E-02	29.99	C350	0 0 0 0 0	
4.509E-04	5.420E-02	35	S203	1 1 2 1 2	
5.555E-04	6.677E-02	39.99	C350	0 0 0 0 0	
4.701E-04	5.650E-02	45	S203	1 1 2 1 2	
6.166E-04	7.412E-02	49.99	C350	0 0 0 0 0	
7.555E-04	9.081E-02	59.99	C350	0 0 0 0 0	
9.221E-04	1.108E-01	69.99	C350	0 0 0 0 0	
1.161E-03	1.395E-01	79.99	C350	0 0 0 0 0	
1.361E-03	1.636E-01	89.99	C350	0 0 0 0 0	
1.616E-03	1.943E-01	99.99	C350	0 0 0 0 0	

1825. C₉H₁₂ClN₅O

Moxonidine

RN: 75438-57-2**MP (°C):****MW:** 241.68**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-03	8.003E-01	ns	R426	0 0 0 0 0	

1826. C₉H₁₂ClO₂PS₃

Carbophenothon-methyl

S-p-Chlorophenylthiomethyl O,O-dimethyl phosphorodithioate

RN: 953-17-3**MP (°C):****MW:** 314.81**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.669E-06	1.470E-03	10	B324	0 0 0 0 0	
4.670E-06	1.470E-03	10	B324	0 0 0 0 0	
5.178E-06	1.630E-03	20	B300	2 1 1 1 2	
5.083E-06	1.600E-03	20	B324	0 0 0 0 0	
5.082E-06	1.600E-03	20	B324	0 0 0 0 0	
8.958E-06	2.820E-03	30	B324	0 0 0 0 0	
8.958E-06	2.820E-03	30	B324	0 0 0 0 0	
3.176E-06	1.000E-03	rt	M161	0 0 0 0 0	

1827. C₉H₁₂ClO₄P

Heptenophos

7-Chlorobicyclo[3.2.0]hepta-2,6-dien-6-yl dimethyl phosphate

Ragadan

Hostaquick

RN: 23560-59-0 **MP (°C):**
MW: 250.62 **BP (°C):** 64

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.975E-03	2.500E+00	23	M161	1 0 0 0 1	

1828. C₉H₁₂Cl₂N₄

2,4-Dichloro-6-cyclohexylamino-1,3,5-triazine

2,4-Dichloro-6-(cyclohexylamino)triazine

1,3,5-Triazin-2-amine, 4,6-dichloro-*N*-cyclohexyl-

RN: 27282-86-6 **MP (°C):**
MW: 247.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.046E-04	1.000E-01	ns	B160	0 0 0 0 2	

1829. C₉H₁₂FN₃O₃

1-Butylcarbamoyl-5-fluorouracil

N-Butyl-5-fluoro-2,4-dioxo-pyrimidinecarboxamide

RN: 64098-82-4 **MP (°C):** 136
MW: 229.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.577E-03	8.200E-01	22	B321	0 0 0 0 0	pH 4.0
3.577E-03	8.200E-01	22	B388	0 0 0 0 0	

1830. C₉H₁₂NO₅PS

Fenitrothion

Dimethyl *O*-(4-nitro-*m*-tolyl) phosphorothioate

Nuvanol

Novathion

Dybar

Metathionine

RN: 122-14-5 **MP (°C):** 3.4
MW: 277.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.089E-05	2.520E-02	20	B169	2 0 1 1 2	
1.396E-04	3.870E-02	22	K137	1 1 2 1 0	<i>sic</i>
1.082E-04	3.000E-02	ns	F071	0 1 2 1 1	
1.082E-04	3.000E-02	ns	M061	0 0 0 0 1	
1.082E-04	3.000E-02	ns	M110	0 0 0 0 0	EFG

1831. C₉H₁₂NO₅PS

O-Methyl O-ethyl O-4-nitrophenyl thiophosphate

Ethylmethylthiophos

Methylethylthiophos

Methylethylthiofos

RN: 2591-57-3

MP (°C):

MW: 277.24

BP (°C): 116

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.443E-04	4.000E-02	ns	M061	0 0 0 0 1	

1832. C₉H₁₂N₂O

Fenuron

3-Phenyl-1,1-dimethylurea

N,N-Dimethyl-N-phenylurea

Beet-Klean

RN: 101-42-8

MP (°C): 133–134

MW: 164.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.344E-02	3.849E+00	20	B179	0 0 0 0 0	
2.245E-02	3.686E+00	20	E048	1 2 1 1 2	
2.253E-02	3.700E+00	20	F311	1 2 2 2 1	
1.766E-02	2.900E+00	24	B185	0 0 0 0 0	
1.761E-02	2.892E+00	24	M061	1 0 0 0 1	
1.462E-02	2.400E+00	25	A039	1 1 0 0 2	
2.345E-02	3.850E+00	25	B200	1 0 0 0 0	
2.345E-02	3.850E+00	25	G036	1 0 0 0 2	
1.462E-02	2.400E+00	25	G099	1 0 0 1 0	
2.452E-02	4.027E+00	25	H073	2 1 1 2 2	
2.345E-02	3.850E+00	25	M161	1 0 0 0 2	
2.426E-02	3.984E+00	ns	B100	0 0 0 0 0	
1.462E-02	2.400E+00	ns	B160	0 0 0 0 2	
2.345E-02	3.850E+00	ns	B185	0 0 0 0 0	
1.761E-02	2.892E+00	ns	N013	0 0 0 0 1	

1833. C₉H₁₂N₂O₂

Dulcin

(4-Ethoxyphenyl)urea

4-Aethoxy-phenylharnstoff

RN: 150-69-6

MP (°C): 173

MW: 180.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.714E-03	1.210E+00	21	F300	1 0 0 0 2	
7.214E-03	1.300E+00	45	F300	1 0 0 0 1	
1.110E-01	2.000E+01	100	F300	1 0 0 0 0	
6.928E-03	1.248E+00	c	I314	0 0 0 0 0	
1.088E-01	1.961E+01	h	I314	0 0 0 0 0	

1834. C₉H₁₂N₂O₂S

3-Thio-2,4-diazaspiro[5.5]undecane-1,3,5-trione
 2,4-Diazaspiro[5.5]undecane-1,5-dione, 3-thioxo-
 2,4-Diazaspiro[5.5]undecane-1,3,5-trione, 3-thio

RN: 52-45-9 **MP (°C):**
MW: 212.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-04	7.323E-02	25	P350	0 0 0 0 0	intrinsic

1835. C₉H₁₂N₂O₃

5-Allyl-5-ethylbarbituric acid
 Barbituric acid, 5-allyl-5-ethyl
 5-Ethyl-5-allylbarbituric acid
 Dormitiv
 5-Ethyl-5-allylbarbiturate

RN: 2373-84-4 **MP (°C):**
MW: 196.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.433E-02	4.774E+00	25	P350	0 0 0 0 0	intrinsic

1836. C₉H₁₂N₂O₃

2,4-Diazaspiro[5.5]undecane-1,3,5-trione
 Spiro[barbituric acid-5,1'-cyclohexane]
 Cyclohexane-spirobarbiturate

RN: 52-44-8 **MP (°C):**
MW: 196.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-04	1.707E-01	25	P350	0 0 0 0 0	intrinsic

1837. C₉H₁₂N₂O₅

Deoxyuridine
RN: 951-78-0 **MP (°C):** 168
MW: 228.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.053E+00	4.685E+02	25.31	T420	0 0 0 0 0	

1838. C₉H₁₂N₂O₆

Uridine

RN: 58-96-8

MP (°C): 166.5

MW: 244.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~3.40E+00	~8.30E+02	21.99	T418	0 0 0 0 0	
~3.20E+00	~7.81E+02	22.99	T418	0 0 0 0 0	

1839. C₉H₁₂N₄O₂

7-Ethyl theophylline

7-Ethyl-1,3-dimethylxanthine

1H-Purine-2,6-dione, 7-ethyl-3,7-dihydro-1,3-dimethyl-

RN: 23043-88-1 MP (°C):

MW: 208.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.760E-01	3.665E+01	30	B042	1 2 1 1 2	
1.760E-01	3.665E+01	30	G021	1 0 0 0 2	

1840. C₉H₁₂N₄O₂

1-Ethyl theobromine

1-Ethyl-3,7-dimethylxanthine

1H-Purine-2,6-dione, 1-ethyl-3,7-dihydro-3,7-dimethyl-

RN: 39832-36-5 MP (°C): 156

MW: 208.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-01	3.977E+01	30	B042	1 2 1 1 2	
1.910E-01	3.977E+01	30	G021	1 0 0 0 2	

1841. C₉H₁₂N₄O₂

1H-Pyrazolo[3,4-d]pyrimidine, 4-(1-ethoxyethoxy)-

1-Ethoxyethyl-4-allopurinyl ether

RN: 52717-51-8 MP (°C):

MW: 208.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.173E-03	1.910E+00	ns	H067	0 0 0 0 0	

1842. C₉H₁₂N₄O₂

8-Methyl caffeine

1,3,7,8-Tetramethylxanthine

RN: 832-66-6 **MP (°C):**
MW: 208.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.045E-02	2.175E+00	20	J009	1 0 2 2 2	

1843. C₉H₁₂N₄O₃

7-β-Hydroxyethyltheophylline

1H-Purine-2,6-dione, 3,7-Dihydro-7-(2-hydroxyethyl)-1,3-dimethyl-

Dilaphyllin

Etofylline

Corophyllin-*N*

RN: 519-37-9 **MP (°C):**
MW: 224.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.439E-01	3.226E+01	ns	J025	0 0 0 0 1	

1844. C₉H₁₂N₄O₃

8-Methoxycaffeine

1H-Purine-2,6-dione, 3,7-dihydro-8-methoxy-1,3,7-trimethyl-

RN: 569-34-6 **MP (°C):**
MW: 224.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-02	2.556E+00	25	K008	1 1 0 1 0	EFG
1.115E-04	2.500E-02	rt	N015	0 0 2 2 1	

1845. C₉H₁₂N₄O₃

1,3,7,9-Tetramethyluric acid

1H-Purine-2,6,8(3H)-trione, 7,9-dihydro-1,3,7,9-tetramethyl-

Temorine

Temurin

Ba 2750

RN: 2309-49-1 **MP (°C):**
MW: 224.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.472E-04	3.300E-02	rt	N015	0 0 2 2 1	

1846. C₉H₁₂N₄O₃S

N4-Acetylulfanilylguanidine

Acetamide, *N*-[4-[[*(*aminoiminomethyl)amino]sulfonyl]phenyl]-*p*-(Guanidinosulfonyl)acetanilide

Sulgin ASG

RN: 19077-97-5 MP (°C):

MW: 256.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-03	3.998E-01	37.50	M142	1 2 0 0 1	
5.766E-02	1.478E+01	h	M142	0 0 0 0 1	

1847. C₉H₁₂O

2,3,5-Trimethyl-phenol

Isopseudocumenol

1-Hydroxy-2,3,5-trimethylbenzene

RN: 697-82-5 MP (°C):

MW: 136.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-03	7.627E-01	25	B316	0 0 0 0 0	

1848. C₉H₁₂O

4-Propylphenol

4-Propyphenol

p-n-Propylphenol

RN: 645-56-7 MP (°C):

MW: 136.20 BP (°C): 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-02	1.427E+00	25	L022	1 0 0 0 0	

1849. C₉H₁₂O

2-Propylphenol

2-*n*-Propylphenol

2-Propyphenol

RN: 644-35-9 MP (°C):

MW: 136.20 BP (°C): 225

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.222E-02	1.664E+00	25	L022	1 0 0 0 0	

1850. C₉H₁₂O

3-Methyl-5-ethyl-phenol
 Phenol, 3-ethyl-5-methyl-
m-Cresol, 5-ethyl-

RN: 698-71-5 **MP (°C):**
MW: 136.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	2.315E+00	25	B316	0 0 0 0 0	

1851. C₉H₁₂O

4-Ethyl-3-methylphenol
 3-Methyl-4-ethylphenol
 4-Ethyl-*m*-cresol

RN: 1123-94-0 **MP (°C):**
MW: 136.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.335E-03	9.990E-01	25	L020	1 0 0 0 0	

1852. C₉H₁₂O

2,4,6-Trimethylphenol
 2-Hydroxymesitylene
 1-Hydroxy-2,4,6-trimethylbenzene
 Mesityl alcohol
 Hydroxymesitylene

RN: 527-60-6 **MP (°C):** 72
MW: 136.20 **BP (°C):** 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-03	1.008E+00	25	B316	0 0 0 0 0	
4.892E-03	6.662E-01	25	L020	1 0 0 0 0	

1853. C₉H₁₂O₂

o-Propoxyphenol
 2-Propoxyphenol
RN: 6280-96-2 **MP (°C):**
MW: 152.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-02	2.359E+00	24.99	B353	0 0 0 0 0	

1854. C₉H₁₂O₂

Cumene hydroperoxide

CHP

RN: 80-15-9

MP (°C):

MW: 152.19

BP (°C): 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.140E-02	1.391E+01	25	K051	1 2 2 1 2	

1855. C₉H₁₂O₂

3-Propoxyphenol

m-Propoxy phenol

Phenol, 3-propoxy-

RN: 16533-50-9

MP (°C):

MW: 152.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.590E-02	3.942E+00	30	B315	0 0 0 0 0	

1856. C₉H₁₂O₂1-*O*-Benzylethanediol

Benzylcellosolve

Benzyl cellosolve

RN: 622-08-2

MP (°C):

MW: 152.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.618E-02	3.984E+00	20	D052	1 1 0 0 0	
2.813E-02	4.282E+00	23	M062	1 0 0 0 1	

1857. C₉H₁₃BrN₂O₂5-Bromo-3-*tert*-butyl-6-methyluracil

Compound 733

RN: 7286-76-2

MP (°C): 188

MW: 261.13

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.570E-03	4.100E-01	25	M061	1 0 0 0 0	
3.121E-03	8.150E-01	ns	B185	0 0 0 0 0	

1858. C₉H₁₃BrN₂O₂

Bromacil

5-Bromo-6-methyl-3,5-butyluracil

RN: 314-40-9 MP (°C): 158.3

MW: 261.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-03	7.100E-01	25	B200	1 0 0 0 2	
3.119E-03	8.143E-01	25	B200	1 0 0 0 2	
3.121E-03	8.150E-01	25	M061	1 0 0 0 2	
3.121E-03	8.150E-01	25	M161	1 0 0 0 2	
3.061E-03	7.994E-01	ns	B100	0 0 0 0 0	

1859. C₉H₁₃ClN₂O₂

Terbacil

3-*tert*-Butyl-5-chloro-6-methyluracil

5-Chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione

Sinbar 80W

Geonter

DPX-D732

RN: 5902-51-2 MP (°C): 176.0

MW: 216.67 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.277E-03	7.100E-01	25	M061	1 0 0 0 2	
3.277E-03	7.100E-01	25	M161	1 0 0 0 2	
3.277E-03	7.100E-01	25	P307	1 0 0 0 1	
3.228E-03	6.995E-01	ns	B100	0 0 0 0 0	

1860. C₉H₁₃ClN₆

Cyanazine

Bladex

2-[[4-Chloro-6-(ethylamino)-1,3,5-triazin-2-yl]amino]-2-methylpropanenitrile

Fortrol

Payze

SD 45418

RN: 21725-46-2 MP (°C): 166.5

MW: 240.70 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.647E-04	1.600E-01	23	B200	1 0 0 0 2	
7.104E-04	1.710E-01	25	B200	1 0 0 0 2	
7.104E-04	1.710E-01	25	M061	1 0 0 0 2	
7.104E-04	1.710E-01	25	M161	1 0 0 0 2	
6.647E-04	1.600E-01	25	S309	1 0 0 0 2	
8.309E-04	2.000E-01	ns	M110	0 0 0 0 0	EFG

1861. C₉H₁₃N

2,4,5-Trimethylaniline

2,4,5-Trimethylanilin

RN: 137-17-7 **MP (°C):**
MW: 135.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.875E-03	1.200E+00	19.40	F300	1 0 0 0 1	
1.109E-02	1.500E+00	28.70	F300	1 0 0 0 1	

1862. C₉H₁₃NO₃

Adrenaline

Adrenalin

Epinephrine

L-1-(3,4-Dihydroxyphenyl)-2-methylaminoethanol

Primatene

Epipen

RN: 51-43-4 **MP (°C):**
MW: 183.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.825E-04	1.800E-01	20	F300	1 0 0 0 1	

1863. C₉H₁₃N₃O₃Orotic acid *n*-butylamideOrotamide, *N*-butyl-

RN: 13156-38-2 **MP (°C):** 276–277
MW: 211.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.700E-02	1.204E+01	–4	N018	0 0 0 0 0	
9.600E-02	2.028E+01	16	N018	0 0 0 0 0	
1.180E-01	2.492E+01	25	N018	0 0 0 0 0	

1864. C₉H₁₃N₃O₃

Zalcitabine

2',3'-Dideoxycytidine

Dideoxycytidine

CCRIS 692

Hivid

DDCYD

RN: 7481-89-2 **MP (°C):** 210–214
MW: 211.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.360E-01	7.098E+01	ns	S469	0 0 0 0 0	

1865. C₉H₁₃N₃O₃

Orotic acid diethylamine
Orotamide, *N,N*-diethyl-

RN: 883-81-8 **MP (°C):** 192–194
MW: 211.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.939E+00	6.208E+02	25	N018	0 0 0 0 0	

1866. C₉H₁₃N₃O₄

Orotic acid isobutanolamine

RN: **MP (°C):** 247–249
MW: 227.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-01	9.543E+01	–4	N018	0 0 0 0 0	
7.060E-01	1.604E+02	16	N018	0 0 0 0 0	
8.410E-01	1.911E+02	25	N018	0 0 0 0 0	

1867. C₉H₁₃N₃O₄

Cytosine deoxyriboside

RN: 951-77-9 **MP (°C):**
MW: 227.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E+00	6.317E+02	25.23	T420	0 0 0 0 0	

1868. C₉H₁₃N₃O₅

Cytidine

RN: 65-46-3 **MP (°C):** > 215
MW: 243.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~9.70E-01	~2.36E+02	21.99	T418	0 0 0 0 0	
~8.00E-01	~1.95E+02	22.99	T418	0 0 0 0 0	

1869. C₉H₁₃N₃O₅

Orotic acid 2-amide-2-methyl-1,3-propanediol

RN: **MP (°C):** 214–215
MW: 243.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-01	8.391E+01	–4	N018	0 0 0 0 0	
5.860E-01	1.425E+02	16	N018	0 0 0 0 0	
6.970E-01	1.695E+02	25	N018	0 0 0 0 0	

1870. C₉H₁₃N₅O₄

Ganciclovir

2-Amino-1,9-dihydro-9-((2-hydroxy-1-(hydroxymethyl)ethoxy)methyl)-6H-purin-6-one

DHPG

RN: 82410-32-0 **MP (°C):** 250**MW:** 255.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-02	3.600E+00	25	B360	0 0 0 0 0	
1.230E-02	3.139E+00	25	Z407	0 0 0 0 0	

1871. C₉H₁₃O₂P

Mesitylene phosphinous acid

Phosphinic acid, (2,4,6-trimethylphenyl)-

RN: 6781-97-1 **MP (°C):** 147.0**MW:** 184.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.565E-02	2.882E+00	1	C061	2 2 2 1 2	
1.619E-02	2.981E+00	25	C061	2 2 2 1 2	
1.754E-02	3.230E+00	35	C061	2 2 2 1 2	
2.082E-02	3.835E+00	45	C061	2 2 2 1 2	
2.836E-02	5.223E+00	65	C061	2 2 2 1 2	
3.774E-02	6.951E+00	85	C061	2 2 2 1 2	

1872. C₉H₁₃O₆PS

Endothion

O,O-Dimethyl S-(5-methoxypyronyl-2-methyl) thiophosphate

RN: 2778-04-3 **MP (°C):** 90.5**MW:** 280.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.141E+00	6.000E+02	ns	M061	0 0 0 0 2	
5.353E+00	1.500E+03	ns	M161	0 0 0 0 1	

1873. C₉H₁₄ClN₅

Cyprozine

2-Chloro-4-cyclopropylamino-6-isopropylamino-1,3,5-triazine

RN: 22936-86-3 **MP (°C):** 167**MW:** 227.70 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.030E-05	6.900E-03	25	B200	1 0 0 0 1	
8.582E-04	1.954E-01	40	B200	1 0 0 0 2	

1874. C₉H₁₄N₂O₃5-Ethyl-5-*n*-propylbarbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-propyl-

5-Ethyl-5-propylbarbiturate

RN: 33376-25-9 **MP (°C):** 146.5**MW:** 198.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.872E-02	5.694E+00	25	B065	1 2 1 1 1	
3.610E-02	7.156E+00	25	M310	2 2 2 2 2	

1875. C₉H₁₄N₂O₃

Metharbital

5,5'-Diethyl-1-methylbarbituric acid

RN: 50-11-3 **MP (°C):** 155**MW:** 198.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.009E-02	2.000E+00	25	B011	2 0 0 1 0	
9.980E-03	1.978E+00	25	B065	1 1 1 1 1	
1.150E-02	2.280E+00	25	G003	1 1 1 1 2	pH 4.7
6.054E-03	1.200E+00	25	P061	0 0 0 0 0	
4.979E-03	9.870E-01	rt	M161	0 0 0 0 2	

1876. C₉H₁₄N₂O₃

Probarbital

5-Ethyl-5-isopropylbarbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(1-methylethyl)

RN: 76-76-6 **MP (°C):** 197.5**MW:** 198.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.104E-03	1.210E+00	25	B065	1 1 1 1 1	
7.111E-03	1.410E+00	25	P350	0 0 0 0 0	intrinsic
1.210E-01	2.399E+01	40	N008	1 0 1 1 2	sic

1877. C₉H₁₄N₆

6-Amino-4-(diallylamino)-1,2-dihydro-1-hydroxy-2-imino-s-triazine

RN: **MP (°C):****MW:** 206.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.459E-01	3.010E+01	37	H004	0 0 0 0 0	

1878. C₉H₁₄O₆

L-Camphoronic acid

L-Camphoronsaeure

RN: 2385-74-2

MP (°C):

MW: 218.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.087E-01	1.110E+02	16	F300	1 0 0 0 2	

1879. C₉H₁₄O₆

Triacetin

Propane-1,2,3-triyl triacetate

Enzactin

Vanay

Triacetylglycerol

Glycerol triacetate

RN: 102-76-1

MP (°C): -78

MW: 218.21

BP (°C): 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.290E-01	7.180E+01	15	F300	1 0 0 0 2	
2.389E-01	5.213E+01	24.50	O005	1 0 2 2 1	
3.118E-02	6.803E+00	ns	F014	0 0 0 0 2	

1880. C₉H₁₅Br₆O₄P

Tris-BP

tris(2,3-Dibromopropyl) phosphate

2,3-Dibromo-1-propanol phosphate (3:1)

2,3-Dibromopropyl phosphate

Flamex T 23P

Anfram 3PB

RN: 126-72-7

MP (°C): 5.5

MW: 697.65

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.147E-05	8.000E-03	24	H116	2 1 0 0 2	

1881. C₉H₁₅Cl₆O₄P

Fyrol FR-2

tris(1,3-Dichloroisopropyl) phosphate

TCPP

Emulsion 212

TDCPP

PF 38

RN: 13674-87-8 **MP (°C):****MW:** 430.91 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.624E-05	7.000E-03	24	H116	2 1 0 0 2	

1882. C₉H₁₅NO₃

Ecgonine

L-Ekgonin

3-Hydroxy-2-tropane carboxylic acid

RN: 481-37-8 **MP (°C):** 198**MW:** 185.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.610E-01	1.780E+02	ns	F300	0 0 0 0 2	

1883. C₉H₁₅NO₃S

Captopril

1-((2S)-3-mercaptop-2-methylpropionyl)-L-proline

Acenorm

Capoten

Capozide

(S)-1-(3-Mercapto-2-methyl-1-oxopropyl)-L-proline

RN: 62571-86-2 **MP (°C):****MW:** 217.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.602E-01	1.000E+02	ns	K444	0 0 0 0 0	
6.348E-01	1.379E+02	ns	S469	0 0 0 0 0	

1884. C₉H₁₆

2,2,5-Trimethyl-3-hexyne

3-Hexyne, 2,2,5-trimethyl-

RN: 17530-23-3 **MP (°C):****MW:** 124.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.410E-04	2.994E-02	25	H039	1 2 2 2 2	

1885. C₉H₁₆

1-Nonyne

n-Heptylacetylene

Heptylacetylene

RN: 3452-09-3 MP (°C): -50

MW: 124.23 BP (°C): 150

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.796E-05	7.200E-03	25	M001	2 1 2 2 1	

1886. C₉H₁₆ClN₄

G 30451

2-Chloro-4-propylamino-6-isopropylamino-*s*-triazine

RN: 3567-85-9 MP (°C):

MW: 215.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.947E-04	4.200E-02	21	B192	0 0 0 0 1	

1887. C₉H₁₆ClN₅

Propazine

2-Chloro-4-isopropylamino-6-isopropylamino-*s*-triazine

RN: 139-40-2 MP (°C): 213

MW: 229.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.744E-05	8.600E-03	20	B185	0 0 0 0 0	
4.000E-05	9.189E-03	20	B200	1 0 0 0 0	
2.307E-05	5.300E-03	20	C048	2 2 2 2 1	
2.177E-05	5.000E-03	20	F311	1 2 2 2 1	
3.744E-05	8.600E-03	20	M161	1 0 0 0 1	
3.744E-05	8.600E-03	21	B192	0 0 0 0 1	
3.744E-05	8.600E-03	21	G099	2 0 0 1 0	
3.744E-05	8.600E-03	22	M061	1 0 0 0 1	
7.700E-05	1.769E-02	50	G001	1 0 1 1 1	
3.744E-05	8.600E-03	ns	C101	0 0 0 0 1	
4.353E-05	1.000E-02	ns	G041	0 0 0 0 1	
3.744E-05	8.600E-03	ns	J033	0 0 0 0 0	

1888. C₉H₁₆ClN₅

Terbutylazine

Terbutylazine

2-Chloro-4-ethylamino-6-*tert*-butylamino-*s*-triazine

Primatol M

RN: 5915-41-3 **MP (°C):** 178**MW:** 229.71 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.177E-05	5.000E-03	20	F311	1 2 2 2 1	
3.700E-05	8.500E-03	20	M161	1 0 0 0 1	
3.700E-05	8.500E-03	ns	J033	0 0 0 0 0	

1889. C₉H₁₆ClN₅

Trietazine

2-Chloro-4-diethylamino-6-ethylamino-*s*-triazine2-Chloro-4-ethylamino-6-diethylamino-*s*-triazines**RN:** 1912-26-1 **MP (°C):** 101**MW:** 229.71 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.706E-05	2.000E-02	20	B185	0 0 0 0 0	
8.706E-05	2.000E-02	21	B192	0 0 0 0 1	
8.706E-05	2.000E-02	21	G099	2 0 0 1 0	
8.706E-05	2.000E-02	25	M161	1 0 0 0 1	
8.706E-05	2.000E-02	ns	J033	0 0 0 0 0	

1890. C₉H₁₆N₂O₄

Methyl-2,2-diethylmalonurate

Methyl 2,2-diethylmalonurate

RN: 69577-07-7 **MP (°C):** 112**MW:** 216.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-02	2.379E+00	23	B152	1 2 1 1 1	pH 3.5

1891. C₉H₁₆N₄OS

Tebuthiuron

1-(5-*tert*-Butyl-1,3,4-thiadiazol-2-yl)-1,3-dimethylurea

Graslan

Spike

Spike 20P

Perflan

RN: 34014-18-1 **MP (°C):** 162.2**MW:** 228.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.007E-02	2.300E+00	ns	M161	0 0 0 0 1	

1892. C₉H₁₆N₈2-Azido-4-ethylamino-4-*t*-butylamino-*s*-triazine

WL 9385

RN: 2854-70-8 MP (°C): 102.5

MW: 236.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.047E-04	7.200E-02	20	M061	1 0 0 0 1	

1893. C₉H₁₆O₂

3-Hydroxy-5-spirocyclohexyltetrahydrofuran

1-Oxaspiro[4.5]decan-3-ol

RN: 29839-61-0 MP (°C):

MW: 156.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.255E-01	1.961E+01	rt	B066	0 2 0 0 0	contains impurity

1894. C₉H₁₆O₂

g-Nonanolactone

4-Hydroxynonanoic acid lactone

g-*n*-Amylbutyrolactone

g-Pentyl-g-butyrolactone

g-Nonanolide

RN: 104-61-0 MP (°C):

MW: 156.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-02	9.217E+00	25	D407	1 0 2 2 2	
5.902E-02	9.221E+00	ns	S460	0 0 0 0 0	

1895. C₉H₁₆O₂

3-Hydroxy-2-methyl-5-spirocyclopentyltetrahydrofuran

1-Oxaspiro[4.4]nonan-3-ol, 2-methyl-

RN: 29839-62-1 MP (°C):

MW: 156.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.067E+00	1.667E+02	rt	B066	0 2 0 0 1	

1896. C₉H₁₆O₄

Butyl α-acetoxypropionate

Hydracrylic acid, butyl ester, acetate

RN: 5422-69-5 MP (°C):

MW: 188.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	3.200E+00	25	R006	2 2 0 1 1	

1897. C₉H₁₆O₄

Azelaic acid

Azelainsaeure

Nonanedioic acid

RN: 123-99-9 MP (°C): 106.5

MW: 188.23 BP (°C): 287

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.313E-03	1.000E+00	0	L041	1 0 0 1 1	
3.298E-03	6.208E-01	6.99	A340	0 0 0 0 0	
4.513E-03	8.494E-01	12.69	A340	0 0 0 0 0	
7.969E-03	1.500E+00	15	L041	1 0 0 1 1	
6.475E-03	1.219E+00	18.69	A340	0 0 0 0 0	
1.275E-02	2.400E+00	20	F300	1 0 0 0 1	
1.275E-02	2.400E+00	20	L041	1 0 0 1 1	
1.297E-02	2.441E+00	20	M171	1 0 0 0 1	
2.667E-01	5.020E+01	21	B040	1 0 1 1 2	sic
9.461E-03	1.781E+00	24.99	A340	0 0 0 0 0	
1.589E-02	2.990E+00	34.69	A340	0 0 0 0 0	
2.391E-02	4.500E+00	35	L041	1 0 0 1 1	
1.858E-02	3.498E+00	42.99	A340	0 0 0 0 0	
4.356E-02	8.200E+00	50	L041	1 0 0 1 1	
2.662E-02	5.010E+00	52.59	A340	0 0 0 0 0	
3.858E-02	7.263E+00	56.99	A340	0 0 0 0 0	
5.124E-02	9.645E+00	61.49	A340	0 0 0 0 0	
7.023E-02	1.322E+01	64.99	A340	0 0 0 0 0	
1.169E-01	2.200E+01	65	F300	1 0 0 0 1	
1.169E-01	2.200E+01	65	L041	1 0 0 1 1	
7.255E-02	1.366E+01	70.99	A340	0 0 0 0 0	
8.355E-02	1.573E+01	74.49	A340	0 0 0 0 0	
1.048E-01	1.972E+01	79.89	A340	0 0 0 0 0	
9.430E-02	1.775E+01	84.49	A340	0 0 0 0 0	
9.440E-03	1.777E+00	rt	H431	0 0 0 0 0	

1898. C₉H₁₆O₅

Propanoic acid, 2-[(butoxycarbonyl)oxy]-, methyl ester
 Propanoic acid, 2-[(methoxycarbonyl)oxy]-, butyl ester

RN: MP (°C):
MW: 204.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.798E-03	1.797E+00	25	R007	0 0 0 0 0	

1899. C₉H₁₇ClN₃O₃PS

Isazophos
 Diethyl *O*-(5-chloro-1-(1-methylethyl)-1H-1,2,4-triazol-3-yl) phosphorothioate
 Miral

Triumph
 CGA-12223
RN: 42509-80-8 **MP (°C):**
MW: 313.74 **BP (°C):** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E-04	1.500E-01	20	E048	1 2 1 1 2	
4.781E-04	1.500E-01	20	M161	1 0 0 0 1	

1900. C₉H₁₇NOS

Molinate
 S-Ethyl hexahydro-1H-azepine-1-carbothioate
 Hydram
 Carbothialate, ethyl-1-hexa-methylene imine-
 Poperidinecarbothioic acid, *S*-ethyl ester

RN: 2212-67-1 **MP (°C):**
MW: 187.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.271E-03	8.000E-01	20	B200	1 0 0 0 2	
4.271E-03	8.000E-01	21	M161	1 0 0 0 2	
4.698E-03	8.800E-01	22	K137	1 1 2 1 0	
4.698E-03	8.800E-01	25	P434	0 0 0 0 0	
<5.33E-03	<9.99E-01	ns	B185	0 0 0 0 0	
4.869E-03	9.120E-01	ns	F019	0 0 0 0 2	
5.334E-03	9.990E-01	ns	M061	0 0 0 0 0	

1901. C₉H₁₇NO₃

Diethylaceturethane

Detonal

RN: MP (°C):
MW: 187.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.796E-02	5.236E+00	ns	O021	0 2 0 0 0	

1902. C₉H₁₇NO₄

3,3-Dihydroxy-2,2,5,5-tetramethyl-4-carbamyltetrahydrofuran

3-Furamide, tetrahydro-4,4-dihydroxy-2,2,5,5-tetramethyl-

RN: 29839-68-7 MP (°C):
MW: 203.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.473E-01	9.091E+01	rt	B066	0 2 0 0 1	

1903. C₉H₁₇N₅O

Atratone

2-Methoxy-4-ethylamino-6-isopropylamino-s-triazine

2-Methoxy-4-ethylamino-6-isopropylamino-s-triazines

RN: 1610-17-9 MP (°C):
MW: 211.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.520E-03	1.800E+00	20	B185	0 0 0 0 0	
8.520E-03	1.800E+00	20	M061	1 0 0 0 2	
8.520E-03	1.800E+00	21	B192	0 0 0 0 2	
8.520E-03	1.800E+00	21	G099	2 0 0 1 0	
7.905E-03	1.670E+00	25	H073	2 1 1 2 2	
1.240E-02	2.620E+00	50	G001	1 0 1 1 2	
9.448E-03	1.996E+00	ns	B100	0 0 0 0 0	
8.520E-03	1.800E+00	ns	C101	0 0 0 0 1	
7.829E-03	1.654E+00	ns	J033	0 0 0 0 0	

1904. C₉H₁₇N₅S

Ametryn

(2-Methylthio-4-ethylamino-6-isopropylamino-s-triazine

Ametryne

N-Ethyl-N'-(1-methylethyl)-6-(methylthio)-1,3,5-triazine-2,4-diamine

Ametrex

RN: 834-12-8 MP (°C): 84

MW: 227.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-04	1.841E-01	20	B200	1 0 0 0 1	
8.358E-04	1.900E-01	20	F311	1 2 2 2 1	
8.138E-04	1.850E-01	20	M161	1 0 0 0 2	
9.194E-04	2.090E-01	25	H073	2 1 1 2 2	
1.660E-03	3.774E-01	50	G001	1 0 1 1 2	
8.138E-04	1.850E-01	ns	C101	0 0 0 0 1	
8.490E-04	1.930E-01	ns	J033	0 0 0 0 0	

1905. C₉H₁₈

1-Nonene

α-Nonene

1-*n*-Nonene*n*-Non-1-ene

RN: 124-11-8 MP (°C): -81

MW: 126.24 BP (°C): 146.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.850E-06	1.117E-03	25	M342	1 0 1 1 2	

1906. C₉H₁₈

1,1,3-Trimethylcyclohexane

Cyclogeraniolane

RN: 3073-66-3 MP (°C): -65.7

MW: 126.24 BP (°C): 136.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-05	1.770E-03	25	K119	1 0 0 0 2	
1.402E-05	1.770E-03	25	P051	2 1 1 2 2	
1.402E-05	1.770E-03	25.00	P007	2 1 2 2 2	

1907. C₉H₁₈N₂O₂S

Thiofanox

3,3-Dimethyl-1-(methylthio)-2-butanone *O*-((methylamino)carbonyl)oxime

Thiophanox

DS-15647

Dacamox

RN: 39196-18-4 **MP (°C):** 57
MW: 218.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.382E-02	5.200E+00	22	M161	1 0 0 0 1	

1908. C₉H₁₈N₂O₄

Meprobamate

2-Methyl-2-propyl-1,3-propanediol dicarbamate

Deprol

Meprospan

Miltown

Pathibamate

RN: 57-53-4 **MP (°C):** 104
MW: 218.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.841E-02	6.200E+00	25	C039	1 2 2 1 1	form II
1.512E-02	3.300E+00	25	C039	1 2 2 1 1	form I
1.512E-02	3.300E+00	25	D082	1 0 1 0 1	
3.757E-02	8.200E+00	30	C039	1 2 2 1 1	form II
1.970E-02	4.300E+00	30	C039	1 2 2 1 1	form I
2.612E-02	5.700E+00	35	C039	1 2 2 1 1	form I
4.857E-02	1.060E+01	35	C039	1 2 2 1 2	form II
3.391E-02	7.400E+00	40	C039	1 2 2 1 1	form I
5.865E-02	1.280E+01	40	C039	1 2 2 1 2	form II

1909. C₉H₁₈N₃S₆Fe

Ferbam

tris(Dimethyldithiocarbamate)iron

Knockmate

Ferbeck

Hexaferb

Trifungol

RN: 14484-64-1 **MP (°C):**
MW: 416.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.881E-04	1.200E-01	rt	I314	0 0 0 0 0	
3.121E-04	1.300E-01	rt	M161	0 0 0 0 2	

1910. C₉H₁₈N₆

Altretamine

Hexamethylmelamine

2,4,6-tris(Dimethylamino)-1,3,5-triazine

HMM

Hexastat

Hemel

RN: 645-05-6 MP (°C): 172.0

MW: 210.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.846E-04	8.088E-02	25	B386	0 0 0 0 0	
4.327E-04	9.100E-02	25	C051	1 2 1 1 1	pH 7
4.150E-04	8.727E-02	25	K043	2 0 0 0 0	extrapolated

1911. C₉H₁₈N₆1,3,5-Triazine-2,4,6-triamine, *N,N',N''-Triethyl-**N₂,N₄,N₆-Triethylmelamine*

tris(Ethylamino)-1,3,5-triazine

2,4,6-tris(Ethylamino)-1,3,5-triazine

2,4,6-tris(Ethylamino)-*s*-triazine*N,N',N''-Triethyl-1,3,5-triazine-2,4,6-triamine*

RN: 16268-92-1 MP (°C):

MW: 210.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.318E-03	1.539E+00	25	B386	0 0 0 0 0	

1912. C₉H₁₈N₆O

N-Methylolpentamethylmelamine

N-(Hydroxymethyl)pentamethylmelamine

(Hydroxymethyl)pentamethylmelamine

RN: 16269-01-5 MP (°C): 121.0

MW: 226.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.977E-03	9.000E-01	25	C051	1 2 1 1 0	pH 7, unstable in water

1913. C₉H₁₈N₆OEthanol, 2-[[4,6-bis(dimethylamino)-*s*-triazin-2-yl]amino]-

Ethanol, 2-[[4,6-bis(dimethylamino)-1,3,5-triazin-2-yl]amino]-

RN: 31482-09-4 MP (°C):

MW: 226.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.132E-02	2.562E+00	25	B386	0 0 0 0 0	

1914. C₉H₁₈N₆O₃

N2,N4,N6-Trimethyl-N2,N4,N6-trimethylolmelamine

N,N',N"-Trimethyl-N,N',N"-trimethylolmelamine

Trimelamol

CB 10-375

RN: 64124-21-6 MP (°C): 129

MW: 258.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-02	9.040E+00	25	C051	1 2 1 1 2	pH 7

1915. C₉H₁₈O

Nonyl aldehyde

n-Nonanal

RN: 124-19-6 MP (°C):

MW: 142.24 BP (°C): 93

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.749E-04	9.600E-02	25	A049	1 0 0 0 1	

1916. C₉H₁₈O

5-Nonanone

Dibutyl ketone

RN: 502-56-7 MP (°C): -50

MW: 142.24 BP (°C): 186.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-03	5.078E-01	10	G032	1 2 1 1 2	
1.800E-03	2.560E-01	25	K012	1 0 0 0 1	
2.550E-03	3.627E-01	30	G032	1 2 1 1 2	
2.430E-03	3.457E-01	50	G032	1 2 1 1 2	

1917. C₉H₁₈O

3-Hydroxy-2,3,4,5,5-pentamethyltetrahydrofuran

RN: MP (°C):

MW: 142.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.391E-01	9.091E+01	rt	B066	0 2 0 0 1	

1918. C₉H₁₈O

2,6-Dimethyl-4-heptanone

Diisobutyl ketone

RN: 108-83-8

MP (°C):

MW: 142.24

BP (°C): 169

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.851E-02	2.633E+00	23.50	O005	2 0 2 2 2	

1919. C₉H₁₈O

2-Nonanone

Nonan-2-one

RN: 821-55-6

MP (°C): -21

MW: 142.24

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-03	1.900E-01	25	L450	0 0 0 0 0	

1920. C₉H₁₈O₂

3-Hydroxy-2-isopropyl-5,5-dimethyltetrahydrofuran

3-Furanol, tetrahydro-2-isopropyl-5,5-dimethyl-

RN: 29839-66-5 MP (°C):

MW: 158.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.009E-01	4.762E+01	rt	B066	0 2 0 0 0	

1921. C₉H₁₈O₂

Pelargonic acid

1-Octanecarboxylic acid

Nonylic acid

n-Nonanoic acid

RN: 112-05-0 MP (°C): 12

MW: 158.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.847E-04	1.400E-01	0	B136	1 0 2 1 1	
1.795E-03	2.840E-01	20	B136	1 0 2 1 2	
1.643E-03	2.599E-01	20.0	R001	1 1 1 1 1	
2.003E-03	3.170E-01	30	B136	1 0 2 1 2	
1.340E-03	2.120E-01	30	E005	2 1 1 2 2	
2.022E-03	3.199E-01	30.0	R001	1 1 1 1 1	
2.496E-03	3.950E-01	40	B136	1 0 2 1 2	
1.403E-03	2.220E-01	40	E005	2 1 1 2 2	
2.591E-03	4.100E-01	45	B136	1 0 2 1 1	
2.590E-03	4.098E-01	45.0	R001	1 1 1 1 1	

(continued)

1921. C₉H₁₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E-03	2.640E-01	50	E005	2 1 1 2 2	
3.223E-03	5.100E-01	60	B136	1 0 2 1 1	
1.890E-03	2.990E-01	60	E005	2 1 1 2 2	
3.221E-03	5.097E-01	60.0	R001	1 1 1 1 1	
8.846E-04	1.400E-01	.0	R001	1 1 1 1 1	

1922. C₉H₁₈O₂

Methyl octanoate

Methyl caprylate

Methyl octylate

RN: 111-11-5

MP (°C): -37

MW: 158.24

BP (°C): 194.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.069E-04	6.440E-02	20	M337	2 1 2 2 2	

1923. C₉H₁₈O₂

3-Hydroxy-5-propyl-2,5-dimethyltetrahydrofuran

3-Furanol, 2,5-dimethyltetrahydro-5-propyl-

RN: MP (°C):

MW: 158.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.841E-01	2.913E+01	rt	B066	0 2 0 0 0	

1924. C₉H₁₈O₂

3-Hydroxy-5-methyl-5-isobutyltetrahydrofuran

3-Furanol, 5-isobutyltetrahydro-5-methyl-

RN: MP (°C):

MW: 158.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.257E-02	9.901E+00	rt	B066	0 2 0 0 0	

1925. C₉H₁₈O₂

3-Hydroxy-5-methyl-5-butyltetrahydrofuran

3-Furanol, 5-butyltetrahydro-5-methyl-

RN: MP (°C):

MW: 158.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.518E-02	3.984E+00	rt	B066	0 2 0 0 0	

1926. C₉H₁₈O₂

3-Hydroxy-3-ethyl-2,2,5-trimethyltetrahydrofuranol
 3-Furanol, 3-ethyltetrahydro-2,2,5-trimethyl-

RN: 29839-58-5 **MP (°C):**
MW: 158.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.134E-01	6.542E+01	rt	B066	0 2 0 0 0	

1927. C₉H₁₈O₂

3-Hydroxy-2-methyl-2,5-diethyltetrahydrofuran
 3-Furanol, 2,5-diethyltetrahydro-2-methyl-

RN: 29839-64-3 **MP (°C):**
MW: 158.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-01	1.961E+01	rt	B066	0 2 0 0 0	

1928. C₉H₁₈O₂

3-Hydroxy-2,2,4,5,5-pentamethyltetrahydrofuran
 3-Furanol, tetrahydro-2,2,4,5,5-pentamethyl-

RN: 29839-76-7 **MP (°C):**
MW: 158.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.257E-02	9.901E+00	rt	B066	0 2 0 0 0	

1929. C₉H₁₈O₂

Butyl valerate
n-Butyl pentanoate
 Butyl valerianate

RN: 591-68-4 **MP (°C):**
MW: 158.24 **BP (°C):** 186–187

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	8.387E-02	25	K012	1 0 0 0 1	

1930. C₉H₁₈O₂

Pentyl butyrate
n-Amyl *n*-butyrate
 Pentyl *n*-butanoate

RN: 540-18-1 **MP (°C):**
MW: 158.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	1.741E-01	20	S006	1 0 0 0 1	

1931. C₉H₁₈O₂

3-Hydroxy-2-methyl-5,5-diethyltetrahydrofuran

3-Furanol, 5,5-diethyltetrahydro-2-methyl-

RN: 6744-54-3 **MP (°C):****MW:** 158.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.144E-02	4.975E+00	rt	B066	0 2 0 0 0	

1932. C₉H₁₈O₃

2,2-Diethyl-5-methyl-tetrahydrofuran-3,4-diol

3,4-Furandiol, 2,2-diethyltetrahydro-5-methyl-

RN: 31889-35-7 **MP (°C):****MW:** 174.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.565E-01	1.667E+02	rt	B066	0 2 0 0 1	

1933. C₉H₁₈O₃*n*-Propyl β-*n*-propoxypropionate

Propanoic acid, 3-propoxy-, propyl ester

RN: 14144-41-3 **MP (°C):****MW:** 174.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.059E-02	3.587E+00	25	R034	0 0 0 0 1	

1934. C₉H₁₈O₃*n*-Amyl β-methoxypropionate

Pentyl 3-methoxypropionate

RN: 10500-16-0 **MP (°C):****MW:** 174.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-02	2.892E+00	25	R034	0 0 0 0 1	

1935. C₉H₁₈O₃

1,3-Dioxolane-4-methanol, 2-butyl-2-methyl

RN: 5694-76-8 **MP (°C):****MW:** 174.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-01	3.380E+01	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

1936. C₉H₁₈O₃*n*-Butyl β-ethoxypropionate

Propionic acid, 3-ethoxy-, butyl ester

RN: 14144-35-5 MP (°C):

MW: 174.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.287E-02	3.984E+00	25	D002	1 2 1 1 1	

1937. C₉H₁₈O₃

Hexyl lactate

Propanoic acid, 2-hydroxy-, hexyl ester

RN: 20279-51-0 MP (°C):

MW: 174.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-02	2.700E+00	25	R006	2 2 0 1 1	

1938. C₉H₁₉NOS

Eptam

EPTC

Ethyl *N,N'*-di-*n*-propylthiocarbamate*S*-Ethyl dipropylthiocarbamate*S*-Ethyl *N,N*-di-*n*-propylthiocarbamate

RN: 759-94-4 MP (°C): <25

MW: 189.32 BP (°C): 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.359E-03	6.360E-01	3	G319	0 0 0 0 0	
1.954E-03	3.700E-01	20	B200	1 0 0 0 2	
1.981E+01	3.750E+03	20	F019	1 0 0 0 2	<i>sic</i>
1.981E-03	3.750E-01	20	M061	1 0 0 0 2	
1.928E-03	3.650E-01	20	M161	1 0 0 0 2	
4.170E+00	7.895E+02	25	B185	0 0 0 0 0	<i>sic</i>
1.981E-03	3.750E-01	25	G319	0 0 0 0 0	
1.981E-03	3.750E-01	25	M131	0 0 0 0 2	
2.123E-03	4.020E-01	28	H109	1 0 0 0 2	
1.981E-03	3.750E-01	ns	V414	0 0 0 0 0	

1939. C₉H₁₉NO₂*n*-Octyl carbamate

Carbamic acid, octyl ester

RN: 2029-64-3 MP (°C): 67

MW: 173.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	8.663E-02	37	H006	1 2 2 1 0	

1940. C₉H₁₉O₃

3-Hydroxy-4-methylol-2,2,5,5-tetramethyltetrahydrofuran

RN: MP (°C):

MW: 175.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.119E-01	1.961E+01	rt	B066	0 2 0 0 0	

1941. C₉H₂₀

3,3-Diethylpentane

Tetraethylmethane

RN: 1067-20-5 MP (°C):

MW: 128.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.450E-06	1.212E-03	25	D346	0 0 0 0 0	

1942. C₉H₂₀

2,5-Dimethylheptane

RN: 2216-30-0 MP (°C):

MW: 128.26 BP (°C): 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-06	3.192E-04	ns	S460	0 0 0 0 0	

1943. C₉H₂₀

3-Methyloctane

Octane, 3-methyl-

RN: 2216-33-3 MP (°C):

MW: 128.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.237E-06	8.000E-04	23	C332	0 0 0 0 0	

1944. C₉H₂₀

2-Methyl-4-ethylhexane

RN: 3074-75-7 **MP (°C):**
MW: 128.26 **BP (°C):** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.799E-06	3.590E-04	ns	S460	0 0 0 0 0	

1945. C₉H₂₀

2,2,3-Trimethylhexane

RN: 16747-25-4 **MP (°C):**
MW: 128.26 **BP (°C):** 134

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-06	3.623E-04	ns	S460	0 0 0 0 0	

1946. C₉H₂₀

2,4-Dimethylheptane

RN: 2213-23-2 **MP (°C):**
MW: 128.26 **BP (°C):** 133

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.938E-06	3.768E-04	ns	S460	0 0 0 0 0	

1947. C₉H₂₀

2,2,5-Trimethylhexane

Hexane, 2,2,5-trimethyl-

RN: 3522-94-9 **MP (°C):** -120
MW: 128.26 **BP (°C):** 124.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.159E-06	7.900E-04	0	P003	2 2 2 2 1	
8.966E-06	1.150E-03	25	M001	2 1 2 2 2	
4.210E-06	5.400E-04	25	P003	2 2 2 2 1	

1948. C₉H₂₀

2,2-Dimethylheptane

RN: 1071-26-7 **MP (°C):**
MW: 128.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-06	3.592E-04	ns	S460	0 0 0 0 0	

1949. C₉H₂₀

Nonane

n-Nonan

RN: 111-84-2 **MP (°C):** -53
MW: 128.26 **BP (°C):** 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.72E-05	<2.20E-03	20	M337	2 1 2 2 1	
9.512E-07	1.220E-04	25	K119	1 0 0 0 2	
1.715E-06	2.200E-04	25	M003	1 0 2 2 2	
1.333E-06	1.710E-04	25	T423	0 0 0 0 0	
9.512E-07	1.220E-04	25.0	P051	2 1 1 2 2	
9.512E-07	1.220E-04	25.00	P007	2 1 2 2 2	
2.409E-06	3.090E-04	69.7	P051	2 1 1 2 2	
3.275E-06	4.200E-04	99.1	P051	2 1 1 2 2	
3.275E-06	4.200E-04	99.10	P007	2 1 2 2 2	
1.325E-05	1.700E-03	121.3	P051	2 1 1 2 2	
1.325E-05	1.700E-03	121.30	P007	2 1 2 2 2	
3.953E-05	5.070E-03	136.6	P051	2 1 1 2 2	
3.953E-05	5.070E-03	136.60	P007	2 1 2 2 2	

1950. C₉H₂₀

4,4-Dimethylheptane

RN: 1068-19-5 **MP (°C):**
MW: 128.26 **BP (°C):** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-06	3.335E-04	ns	S460	0 0 0 0 0	

1951. C₉H₂₀

2,6-Dimethylheptane

RN: 1072-05-5 **MP (°C):** -103
MW: 128.26 **BP (°C):** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.594E-06	3.327E-04	ns	S460	0 0 0 0 0	

1952. C₉H₂₀

3,5-Dimethylheptane

RN: 926-82-9 **MP (°C):**
MW: 128.26 **BP (°C):** 136

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-06	3.192E-04	ns	S460	0 0 0 0 0	

1953. C₉H₂₀

3-Ethylheptane

RN: 15869-80-4

MP (°C):

MW: 128.26

BP (°C): 143

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.714E-06	2.198E-04	ns	S460	0 0 0 0 0	

1954. C₉H₂₀

4-Ethylheptane

RN: 2216-32-2

MP (°C):

MW: 128.26

BP (°C): 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.888E-06	2.422E-04	ns	S460	0 0 0 0 0	

1955. C₉H₂₀

2,3-Dimethylheptane

RN: 3074-71-3

MP (°C):

MW: 128.26

BP (°C): 141

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.959E-06	2.512E-04	ns	S420	0 0 0 0 0	

1956. C₉H₂₀

2,3,4-Trimethylhexane

RN: 921-47-1

MP (°C):

MW: 128.26

BP (°C): 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.113E-06	2.711E-04	ns	S460	0 0 0 0 0	

1957. C₉H₂₀

3-Ethyl-2-methylhexane

2-Methyl-3-ethylhexane

RN: 16789-46-1

MP (°C):

MW: 128.26

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.239E-06	2.871E-04	ns	S460	0 0 0 0 0	

1958. C₉H₂₀

3,3-Dimethylheptane

RN: 4032-86-4

MP (°C):

MW: 128.26

BP (°C): 137

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-06	3.028E-04	ns	S460	0 0 0 0 0	

1959. C₉H₂₀

4-Methyloctane

4-Metyllooktan

RN: 2216-34-4

MP (°C): -113

MW: 128.26

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.966E-07	1.150E-04	25	K119	1 0 0 0 2	
8.966E-07	1.150E-04	25	P051	2 1 1 2 2	
8.966E-07	1.150E-04	25.00	P007	2 1 2 2 2	

1960. C₉H₂₀NO₃PS₂

Fostion

FAC 20

O,O-Diethyl S-(N-isopropylcarbamylmethyl) dithiophosphate

Prothoate

RN: 2275-18-5 MP (°C): 24.5

MW: 285.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.761E-03	2.500E+00	20	M161	1 0 0 0 1	

1961. C₉H₂₀O

2,6-Dimethyl-4-heptanol

Diisobutylcarbinol

RN: 108-82-7 MP (°C):

MW: 144.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.925E-03	9.990E-01	25	C093	2 1 1 1 1	

1962. C₉H₂₀O*n*-Nonyl alcohol

Nonanol

RN: 143-08-8 **MP (°C):**
MW: 144.26 **BP (°C):** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.340E-04	1.347E-01	20	H330	0 0 0 0 0	
9.700E-04	1.399E-01	25	K025	2 2 1 1 2	

1963. C₉H₂₀O

3-Ethyl-3-heptanol

RN: 19780-41-7 **MP (°C):**
MW: 144.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.802E-03	5.485E-01	ns	S460	0 0 0 0 0	

1964. C₉H₂₀O

2,6-Dimethyl-3-heptanol

RN: 19549-73-6 **MP (°C):**
MW: 144.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.097E-03	4.468E-01	ns	S460	0 0 0 0 0	

1965. C₉H₂₀O

3-Nonanol

Hexyl ethyl carbinol

Ethyl *n*-hexyl carbinol

RN: 624-51-1 **MP (°C):**
MW: 144.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.999E-03	2.884E-01	ns	J300	0 0 0 0 0	

1966. C₉H₂₀O

3,5,5-Trimethylhexanol

3,5,5-Trimethyl hexanol

Nonylol

3,5,5-Trimethyl-1-hexanol

RN: 3452-97-9 **MP (°C):****MW:** 144.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-03	4.501E-01	20	H330	0 0 0 0 0	
3.099E-03	4.470E-01	ns	J300	0 0 0 0 0	

1967. C₉H₂₀O

Methyl-octyl-alcohol

2-Nonanol

Heptylmethylcarbinol

Methyl *n*-heptyl carbinol**RN:** 628-99-9 **MP (°C):****MW:** 144.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.00E-03	<5.77E-01	25	F044	1 0 0 0 0	

1968. C₉H₂₁N

Tripropylamine

Tri-*n*-propylamine*N,N*-Dipropylpropanamine*N,N*-Dipropyl-1-propanamine**RN:** 102-69-2 **MP (°C):** -93.5**MW:** 143.27 **BP (°C):** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.216E-03	7.473E-01	25.04	V013	2 2 2 2 2	

1969. C₉H₂₁O₂PS₃

Terbufos

O,O-Diethyl *S*-(((1,1-dimethylethyl)thio)methyl) phosphorodithioic acid

Counter 15G

Contraven

ST 100

RN: 13071-79-9 **MP (°C):****MW:** 288.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-05	5.500E-03	19	B169	2 1 1 1 1	
1.758E-05	5.070E-03	24	F179	2 2 2 2 2	
1.907E-05	5.500E-03	ns	B325	0 1 0 0 1	

(continued)

1969. C₉H₂₁O₂PS₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E-05	1.000E-02	ns	M110	0 0 0 0 0	
4.334E-05	1.250E-02	ns	M161	0 0 0 0 0	EFG

1970. C₉H₂₁O₃P

Dibutyl methyl phosphonate

Di-n-butyl methanephosphonate

RN: 2404-73-1 MP (°C):

MW: 208.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.842E-02	8.000E+00	25	B070	1 2 0 1 0	

1971. C₉H₂₁O₃PS₃

S-Ethylsulphinylmethyl O,O-di-isopropyl phosphorodithioate

O,O-Diisopropyl S-[(ethylsulfinyl)methyl] dithiophosphate

Aphidan

PSP 204

IPSP

RN: 5827-05-4 MP (°C):

MW: 304.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.927E-03	1.500E+00	15	M161	1 0 0 0 1	

1972. C₉H₂₁O₃PS₃

Terbufos sulfoxide

Phosphorodithioic acid, S-[[(1,1-dimethylethyl)sulfinyl]methyl] O,O-diethyl ester

RN: 10548-10-4 MP (°C):

MW: 304.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>3.61E-03	>1.10E+00	ns	B325	0 1 0 0 1	

1973. C₉H₂₁O₄P

Tripropyl phosphate

Tri-n-propyl phosphate

RN: 513-08-6 MP (°C):

MW: 224.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	6.951E+00	30	V300	2 2 0 1 0	

1974. C₉H₂₁O₄P

Dibutyl methyl phosphate

Methyl dibutyl phosphate

RN: 7242-59-3 MP (°C):

MW: 224.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.166E-02	7.100E+00	25	B070	1 2 2 1 1	

1975. C₉H₂₁O₄P

Diethyl amyl phosphate

O,O-Diethyl O-pentyl phosphate

Diethyl pentyl phosphate

RN: 20195-08-8 MP (°C):

MW: 224.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.345E-02	7.500E+00	25	B070	1 2 0 1 1	

1976. C₉H₂₁O₄PS₃

Terbufos sulfone

Phosphorodithioic acid, S-[(1,1-dimethylethyl)sulfonyl]methyl] O,O-diethyl ester

Counter sulfone

AC 94320

RN: 56070-16-7 MP (°C):

MW: 320.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-03	4.078E-01	18.50	B169	2 0 1 1 2	
1.273E-03	4.078E-01	ns	B325	0 1 0 0 1	

1977. C₉H₂₂O₄P₂S₄

Ethion

O,O,O,O-Tetraethyl S,S-methylene bisphosphorodithioate

Nialate

Ethanox

Diethion

Hylemox

RN: 563-12-2 MP (°C): -25

MW: 384.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-06	5.700E-04	10	B324	0 0 0 0 0	
1.483E-06	5.702E-04	10	B324	0 0 0 0 0	
2.861E-06	1.100E-03	19.50	B169	2 2 1 1 1	
1.769E-06	6.801E-04	20	B324	0 0 0 0 0	
1.769E-06	6.800E-04	20	B324	0 0 0 0 0	

(continued)

1977. C₉H₂₂O₄P₂S₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-06	7.601E-04	30	B324	0 0 0 0 0	
1.977E-06	7.600E-04	30	B324	0 0 0 0 0	

1978. C₁₀H₄Cl₂O₂

Dichlone

2,3-Dichloro-1,4-naphthalenedione

Phygon XL

Phygon

Phygon paste

USR 604

RN: 117-80-6 MP (°C):
 MW: 227.05 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.404E-07	1.000E-04	25	M161	1 0 0 0 0	
3.083E-05	7.000E-03	ns	B160	0 0 0 0 0	
4.404E-06	1.000E-03	ns	B185	0 0 0 0 0	

1979. C₁₀H₅ClN₂O₄

1-Chloro-2,4-dinitronaphthalene

2,4-Dinitro-1-naphthyl chloride

2,4-Dinitrochloronaphthalene

2,4-Dinitro-1-chloronaphthalene

RN: 2401-85-6 MP (°C): 148
 MW: 252.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-06	1.000E-03	25	M061	1 0 0 0 0	

1980. C₁₀H₅Cl₇

Heptachlor

1,4,5,6,7,8,8-Heptachloro-3 α ,4,7,7 α -tetrahydro-4,7-methano-1H-indene

3-Chlorochlordene

Tetrahydro

Rhodiachlor

3,4,5,6,7,8,8 α -Heptachlorodicyclopentadiene

RN: 76-44-8 MP (°C): 95.5
 MW: 373.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.679E-07	1.000E-04	15	B083	2 2 1 2 2	particle size 5 μ m
4.786E-07	1.787E-04	24.99	K436	0 0 0 0 0	
4.822E-07	1.800E-04	25	B083	2 2 1 2 2	particle size 5 μ m

(continued)

1980. C₁₀H₅Cl₇ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-07	5.600E-05	25	I308	0 0 0 0 0	
1.500E-07	5.600E-05	26.5	P027	1 1 2 2 1	
1.500E-07	5.600E-05	27	M161	0 0 0 0 1	
8.438E-07	3.150E-04	35	B083	2 2 1 2 2	particle size 5 μm
1.313E-06	4.900E-04	45	B083	2 2 1 2 2	particle size 5 μm
8.036E-08	3.000E-05	ns	K138	0 0 0 0 2	
1.875E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG
4.822E-07	1.800E-04	ns	V414	0 0 0 0 0	

1981. C₁₀H₅Cl₇O

Heptachlor epoxide

1,4,5,6,7,8,8-Heptachloro-2,3-epoxy-3α,4,7,7α-tetrahydro-4,7-methanoindan

Hepachlor epoxide

RN: 1024-57-3 MP (°C): 160

MW: 389.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.825E-07	1.100E-04	15	B083	2 2 1 2 2	particle size 5 μm
5.137E-07	2.000E-04	25	B083	2 2 1 2 2	particle size 5 μm
5.137E-07	2.000E-04	25	I308	0 0 0 0 0	
8.990E-07	3.500E-04	25	W025	1 0 2 2 2	
8.990E-07	3.500E-04	26.5	P027	1 1 2 2 1	
8.990E-07	3.500E-04	35	B083	2 2 1 2 2	particle size 5 μm
1.541E-06	6.000E-04	45	B083	2 2 1 2 2	particle size 5 μm
1.798E-06	7.000E-04	ns	M110	0 0 0 0 0	EFG
5.137E-07	2.000E-04	ns	V414	0 0 0 0 0	

1982. C₁₀H₅N₃O₆

1,3,8-Trinitronaphthalene

1,3,8-Trinitronaphthalin

RN: 2364-46-7 MP (°C):

MW: 263.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.840E-05	1.800E-02	15	F300	1 0 0 0 1	

1983. C₁₀H₅N₃O₆

1,4,5-Trinitronaphthalene

1,4,5-Trinitronaphthalin

RN: 2243-95-0 MP (°C):

MW: 263.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.520E-04	4.000E-02	15	F300	1 0 0 0 1	

1984. C₁₀H₆Br₂

2,3-Dibromonaphthalene

Naphthalene, 2,3-dibromo-

RN: 13214-70-5 MP (°C):

MW: 285.98 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.922E-07	5.497E-05	4	D351	1 2 1 1 2	
4.778E-07	1.366E-04	25	D351	1 2 1 1 2	
1.222E-06	3.495E-04	40	D351	1 2 1 1 2	

1985. C₁₀H₆Br₂

1,4-Dibromonaphthalene

Naphthalene, 1,4-dibromo-

RN: 83-53-4 MP (°C): 80–82

MW: 285.98 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.333E-07	1.239E-04	4	D351	1 2 1 1 2	
1.217E-06	3.479E-04	25	D351	1 2 1 1 2	
3.006E-06	8.595E-04	40	D351	1 2 1 1 2	

1986. C₁₀H₆Cl₂

1,4-Dichloronaphthalene

Naphthalene, 1,4-dichloro-

RN: 1825-31-6 MP (°C):

MW: 197.07 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.333E-06	2.628E-04	4	D351	1 2 1 1 2	
4.389E-06	8.649E-04	25	D351	1 2 1 1 2	
1.122E-05	2.212E-03	40	D351	1 2 1 1 2	

1987. C₁₀H₆Cl₄O₃S

Glenbar

O,S-Dimethyl tetrachlorothiophthalate

RN: 3765-57-9 MP (°C): 161

MW: 348.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.437E-06	5.000E-04	22	B200	1 0 0 0 0	
1.034E-06	3.600E-04	ns	M061	0 0 0 0 1	

1988. C₁₀H₆Cl₄O₄

Dimethyl tetrachloroterephthalate

DCPA

RN: 1861-32-1 **MP (°C):** 156
MW: 331.97 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-06	5.000E-04	25	B200	1 0 0 0 0	
<1.51E-06	<5.00E-04	25	M161	1 0 0 0 0	
<1.51E-06	<5.00E-04	ns	B185	0 0 0 0 0	
1.506E-06	5.000E-04	ns	V414	0 0 0 0 0	

1989. C₁₀H₆Cl₆

Chlordene

4,5,6,7,8,8-Hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene

RN: 3734-48-3 **MP (°C):** -62
MW: 338.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.281E-06	7.730E-04	26.70	L071	1 2 0 1 2	

1990. C₁₀H₆Cl₆O

1-Hydroxychlordene

1-Hydroxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene

RN: 2597-11-7 **MP (°C):** 194
MW: 354.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.469E-06	1.231E-03	26.70	L071	1 2 0 1 2	

1991. C₁₀H₆Cl₆O

Chlordene epoxide

2,3-Epoxy-4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-4,7-methanoindene

Chlordene hydroxide

4,7-Methano-1H-inden-1-ol, 4,5,6,7,8,8-hexachloro-3α,4,7,7α-tetrahydro-

RN: 6058-23-7 **MP (°C):** 215
MW: 354.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.829E-06	1.359E-03	26.70	L071	1 2 0 1 2	

1992. C₁₀H₆Cl₆O₂

1-Hydroxychlordene epoxide

1-Hydroxy-2,3-epoxy-4,5,6,7,8,8-hexachloro-3 α ,4,7,7 α -tetrahydro-4,7-methanoindene

RN: 24009-06-1 MP (°C):

MW: 370.88 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.391E-06	2.741E-03	26.70	L071	1 1 1 1 2	

1993. C₁₀H₆Cl₈

cis-Chlordan

(1 α ,2 α ,3 α ,4 β ,7 β ,7 α)-1,2,4,5,6,7,8,8-Octachloro-2,3,3 α ,4,7,7 α -hexahydro-4,7-methano-1H-indene
4,7-Methano-1H-indene 1,2,4,5,6,7,8,8-octachloro-2,3,3 α ,4,7,7 α -hexahydro-, (1 α ,2 α ,3 α ,4 β ,7 β ,7 α)
 α -Chlordan

RN: 5103-71-9 MP (°C):

MW: 409.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1994. C₁₀H₆Cl₈

trans-Chlordan

(1 α ,2 β ,3 α ,4 β ,7 β ,7 α)-1,2,4,5,6,7,8,8-Octachloro-2,3,3 α ,4,7,7 α -hexahydro-4,7-methano-1H-indene
4,7-Methano-1H-indene 1,2,4,5,6,7,8,8-octachloro-2,3,3 α ,4,7,7 α -hexahydro-, (1 α ,2 β ,3 α ,4 β ,7 β ,7 α)
 β -Chlordan

RN: 5103-74-2 MP (°C):

MW: 409.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1995. C₁₀H₆Cl₈

Chlordan

1,2,4,5,6,7,8,8-Octachloro-4,7-methano-3 α ,4,7,7 α -tetrahydroindane

Octachlor

Velsicol 1068

Toxicchlor

Ortho-Klor

RN: 57-74-9 MP (°C): 105

MW: 409.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-07	5.657E-05	24.99	K436	0 0 0 0 0	
4.515E-06	1.850E-03	25	W025	1 0 2 2 2	
1.367E-07	5.600E-05	ns	K138	0 0 0 0 2	

(continued)

1995. C₁₀H₆Cl₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.708E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG
1.367E-07	5.600E-05	ns	S187	0 2 2 1 1	
1.367E-07	5.600E-05	ns	V414	0 0 0 0 0	

1996. C₁₀H₆FN₃O₃

3-Nicotinoyl-5-fluorouracil

RN: MP (°C):

MW: 235.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.148E-02	2.700E+000	22	B332	1 1 0 0 1	pH 4.0

1997. C₁₀H₆N₂O₄

1,8-Dinitronaphthalene

1,8-Dinitronaphthalin

RN: 602-38-0 MP (°C): 107

MW: 218.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.558E-04	3.400E-02	15	F300	1 0 0 0 1	

1998. C₁₀H₆N₂O₄

1,5-Dinitronaphthalene

1,5-Dinitronaphthalin

RN: 605-71-0 MP (°C): 216.5

MW: 218.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.658E-04	5.800E-02	12	F300	1 0 0 0 1	

1999. C₁₀H₆O₈

Pyromellitic acid

1,2,4,5-Benzenetetracarboxylic acid

Benzol-tetracarbonsaeure-(1,2,4,5)

RN: 89-05-4 MP (°C):

MW: 254.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.508E-02	1.400E+01	16	F300	1 0 0 0 2	

2000. C₁₀H₇Br

1-Bromonaphthalene

Naphthalene, 1-bromo-

RN: 90-11-9

MP (°C): 6.2

MW: 207.08

BP (°C): 281.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.383E-05	9.077E-03	4	D351	1 2 1 1 2	
4.733E-05	9.802E-03	10	D351	1 2 1 1 2	
4.500E-05	9.318E-03	21	A057	2 1 2 2 1	
6.444E-05	1.334E-02	25	D351	1 2 1 1 2	
9.166E-05	1.898E-02	40	D351	1 2 1 1 2	
6.000E-05	1.242E-02	ns	L060	0 0 0 0 0	
9.120E-05	1.889E-02	ns	S460	0 0 0 0 0	

2001. C₁₀H₇Br

2-Bromonaphthalene

Naphthalene, 2-bromo-

RN: 580-13-2

MP (°C): 53.5

MW: 207.08

BP (°C): 281.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-05	3.831E-03	4	D351	1 2 1 1 2	
3.883E-05	8.041E-03	25	D351	1 2 1 1 2	
7.611E-05	1.576E-02	40	D351	1 2 1 1 2	
4.000E-05	8.283E-03	ns	L060	0 0 0 0 0	

2002. C₁₀H₇Cl

β-Chloronaphthalene

2-Chloronaphthalene

RN: 91-58-7

MP (°C): 59.5

MW: 162.62

BP (°C): 256

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.15E-06	<1.00E-03	30	M311	1 1 2 2 0	
8.000E-05	1.301E-02	ns	L060	0 0 0 0 0	

2003. C₁₀H₇Cl

1-Chloronaphthalene

α-Chloronaphthalene

1-Naphthyl chloride

RN: 90-13-1

MP (°C): -20

MW: 162.62

BP (°C): 259.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.23E-04	<2.00E-02	ns	L060	0 0 0 0 2	
1.164E-04	1.893E-02	ns	S460	0 0 0 0 0	

2004. C₁₀H₇I

α -Iodonaphthalene
1-Iodonaphthalene

RN: 90-14-2
MW: 254.07

MP (°C):
BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	7.114E-03	ns	L060	0 0 0 0 1	average
2.818E-05	7.161E-03	ns	S460	0 0 0 0 0	

2005. C₁₀H₇NO₂

1-Nitronaphthalene
1-Nitro-naphthalin

RN: 86-57-7
MW: 173.17

MP (°C): 59.5
BP (°C): 304

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.887E-04	5.000E-02	18	F300	1 0 0 0 1	

2006. C₁₀H₇NO₃

1-Nitro-2-naphthol
1-Nitro-naphthol-(2)

RN: 550-60-7
MW: 189.17

MP (°C): 104
BP (°C): 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.057E-03	2.000E-01	20	F300	1 0 0 0 2	

2007. C₁₀H₇NO₃

Kynurenic acid
4-Hydroxy-chinolin-carbonsaeure-(2)

Kynurensaeure

RN: 492-27-3
MW: 189.17

MP (°C): 282.5
BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.715E-02	8.920E+00	100	D041	1 0 0 0 0	
4.969E-03	9.400E-01	100	F300	1 0 0 0 1	

2008. C₁₀H₇N₃O₃

Orotic acid pyridine

RN:**MW:** 217.19**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-01	2.606E+01	16	N018	0 0 0 0 0	

2009. C₁₀H₇N₃S

Thiabendazole

2-(Thiazol-4-yl)benzimidazole

Mintezol

Apl-Luster

Mertect

Tecto

RN: 148-79-8**MP (°C):** 304.5**MW:** 201.25**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.484E-04	5.000E-02	25	M161	1 0 0 0 1	intrinsic

2010. C₁₀H₈

Naphthalene

Naphthalene

Mothballs

Camphor tar

RN: 91-20-3**MP (°C):** 80.2**MW:** 128.18**BP (°C):** 217.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	1.730E-02	4.99	P331	0 0 0 0 0	
1.320E-04	1.692E-02	8.20	M082	1 1 1 2 2	
1.320E-04	1.692E-02	8.20	M151	2 1 2 2 1	
1.320E-04	1.692E-02	8.24	M183	1 2 1 1 2	
1.390E-04	1.782E-02	10	J302	2 1 2 2 2	
1.580E-04	2.025E-02	9.99	P331	0 0 0 0 0	
1.500E-04	1.923E-02	11.50	M082	1 1 1 2 2	
1.500E-04	1.923E-02	11.50	M151	2 1 2 2 2	
1.502E-04	1.925E-02	11.54	M183	1 2 1 1 2	
1.570E-04	2.012E-02	12	S076	2 2 2 2 2	
1.590E-04	2.038E-02	13.40	M082	1 1 1 2 2	
1.590E-04	2.038E-02	13.40	M151	2 1 2 2 2	
1.591E-04	2.039E-02	13.44	M183	1 2 1 1 2	
1.900E-04	2.435E-02	14.99	P331	0 0 0 0 0	
1.716E-03	2.200E-01	15	F300	1 0 0 0 2	sic
1.716E-04	2.200E-02	15	M073	1 0 2 2 1	
1.680E-04	2.153E-02	15.10	M082	1 1 1 2 2	

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2010. C₁₀H₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-04	2.153E-02	15.10	M151	2 1 2 2 2	
1.677E-04	2.150E-02	15.14	M183	1 2 1 1 2	
1.900E-04	2.435E-02	18	S076	2 2 2 2 2	
2.010E-04	2.576E-02	19.30	M082	1 1 1 2 2	
2.010E-04	2.576E-02	19.30	M151	2 1 2 2 2	
2.013E-04	2.581E-02	19.34	M183	1 2 1 1 2	
2.240E-04	2.871E-02	19.99	P331	0 0 0 0 0	
1.748E-04	2.240E-02	20	A050	1 0 1 1 1	
7.412E-04	9.500E-02	20	B318	0 0 0 0 0	EFG
3.000E-04	3.845E-02	20	E009	1 0 0 0 1	
3.000E-04	3.845E-02	20	E025	1 0 2 2 1	
1.900E-04	2.435E-02	20	H306	1 0 1 2 1	
1.272E-04	1.630E-02	20	T301	1 2 2 2 2	
2.400E-04	3.076E-02	22	A413	2 0 2 2 1	
2.645E-04	3.390E-02	22	C413	2 0 2 2 1	
1.638E-04	2.100E-02	22	N311	1 0 1 1 2	
2.255E-04	2.890E-02	22.20	W003	2 2 2 2 2	average of 3
2.341E-04	3.000E-02	23	P332	0 0 0 0 0	
2.341E-04	3.000E-02	23	P339	0 0 0 0 0	
2.300E-04	2.948E-02	23.40	M082	1 1 1 2 2	
2.300E-04	2.948E-02	23.40	M151	2 1 2 2 2	
2.301E-04	2.949E-02	23.44	M183	1 2 1 1 2	
2.380E-04	3.050E-02	24.50	W003	2 2 2 2 2	average of 5
2.630E-04	3.371E-02	24.99	P331	0 0 0 0 0	
2.458E-04	3.150E-02	25	A001	1 2 2 2 2	
2.350E-04	3.012E-02	25	A325	2 1 2 2 2	
2.684E-04	3.440E-02	25	B003	2 2 2 2 2	
2.465E-04	3.160E-02	25	B319	2 0 1 2 2	average of 2
2.442E-04	3.130E-02	25	D337	0 0 0 0 0	
2.715E-04	3.480E-02	25	D406	1 2 2 2 2	
2.442E-04	3.130E-02	25	E004	2 1 2 2 2	
2.620E-04	3.358E-02	25	G047	2 2 2 2 2	
2.520E-04	3.230E-02	25	J302	2 1 2 2 2	
9.750E-05	1.250E-02	25	K001	2 2 2 2 2	
2.300E-04	2.948E-02	25	K123	1 0 2 2 1	
2.497E-04	3.200E-02	25	L332	1 1 1 1 0	
2.653E-04	3.400E-02	25	M040	1 0 0 1 1	
2.550E-04	3.268E-02	25	M058	2 2 2 2 2	
2.473E-04	3.170E-02	25	M064	1 1 2 2 2	
2.472E-04	3.169E-02	25	M071	2 2 2 2 2	
3.121E-04	4.000E-02	25	M073	1 0 2 2 1	
2.620E-04	3.358E-02	25	M123	1 0 0 0 2	
2.575E-04	3.300E-02	25	M130	1 0 0 0 1	
2.390E-04	3.063E-02	25	M342	1 0 1 1 2	
2.497E-04	3.200E-02	25	O320	0 0 0 0 0	
2.575E-05	3.300E-03	25	P340	0 0 0 0 0	
2.356E-04	3.020E-02	25	R042	1 2 2 2 2	

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2010. C₁₀H₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.340E-04	2.999E-02	25	S076	2 2 2 2 2	
1.716E-04	2.200E-02	25	S227	1 2 1 1 1	
2.390E-04	3.063E-02	25	W300	2 2 2 2 2	
2.490E-04	3.192E-02	25.00	M082	1 1 1 2 2	
2.490E-04	3.192E-02	25.00	M151	2 1 2 2 2	
2.472E-04	3.169E-02	25.00	M151	2 1 1 2 2	
6.936E-04	8.890E-02	25.00	P007	2 1 2 2 2	
2.492E-04	3.194E-02	25.04	M183	1 2 1 1 2	
2.510E-04	3.217E-02	25.04	V013	2 2 2 2 2	
2.660E-04	3.409E-02	27.00	M082	1 1 1 2 2	
2.660E-04	3.409E-02	27.00	M151	2 1 2 2 2	
2.666E-04	3.417E-02	27.04	M183	1 2 1 1 2	
2.980E-04	3.820E-02	29.90	W003	2 2 2 2 2	average of 3
3.240E-04	4.153E-02	29.99	P331	0 0 0 0 0	
2.949E-04	3.780E-02	30.30	W003	2 2 2 2 2	average of 3
3.448E-04	4.420E-02	34.50	W003	2 2 2 2 2	average of 2
3.710E-04	4.755E-02	34.99	P331	0 0 0 0 0	
4.112E-04	5.270E-02	39.30	W003	2 2 2 2 2	average of 2
4.360E-04	5.588E-02	39.99	P331	0 0 0 0 0	
4.275E-04	5.480E-02	40.10	W003	2 2 2 2 2	
5.118E-04	6.560E-02	44.70	W003	2 2 2 2 2	average of 3
6.132E-04	7.860E-02	50.20	W003	2 2 2 2 2	
8.270E-04	1.060E-01	55.60	W003	2 2 2 2 2	
1.233E-03	1.580E-01	64.50	W003	2 2 2 2 2	average of 3
1.904E-03	2.440E-01	73.40	W003	2 2 2 2 2	average of 3
2.341E-04	3.000E-02	ns	F071	0 1 2 1 1	
2.341E-04	3.000E-02	ns	H080	0 0 0 0 1	
2.473E-04	3.170E-02	ns	H123	0 0 0 0 0	
2.473E-04	3.170E-02	ns	K304	0 0 0 0 2	
2.340E-04	2.999E-02	ns	L060	0 0 0 0 2	average
2.473E-04	3.170E-02	ns	M344	0 0 0 0 2	
2.341E-04	3.000E-02	ns	O009	0 0 0 0 0	
8.129E-04	1.042E-01	ns	R042	1 2 2 2 2	
2.341E-04	3.000E-02	rt	M161	0 0 0 0 1	
2.848E-04	3.650E-02	rt	S314	0 0 2 1 2	

2011. C₁₀H₈BrN₃O

Bropirimine

2-Amino-5-bromo-6-phenyl-pyrimidin-4(3H)-one

ABPP

RN: 56741-95-8 MP (°C):

MW: 266.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.931E-05	7.800E-03	37	A346	0 0 0 0 0	EFG

2012. C₁₀H₈BrN₃O

Brompyrazone

Amino-4-bromo-2-phenyl-3(2H)-pyridazinone

1-Phenyl-4-amino-5-bromo-6-pyridazone

Pyridazinone, 5-amino-4-bromo-2-phenyl-

RN: 3042-84-0 MP (°C): 223.5

MW: 266.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.516E-04	2.000E-01	20	M161	1 0 0 0 2	

2013. C₁₀H₈ClN₃O

Pyrazon

5-Amino-4-chloro-2-phenyl-3(2H)-pyridazinone

RN: 1698-60-8 MP (°C): 207

MW: 221.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.353E-03	3.000E-01	20	B185	0 0 0 0 0	
1.353E-03	2.999E-01	20	B200	1 0 0 0 0	
1.353E-03	2.999E-01	20	M061	1 0 0 0 0	
1.805E-03	4.000E-01	20	M161	1 0 0 0 2	

2014. C₁₀H₈N₂

γ,γ'-Dipyridyl

4,4'-Bipyridyl

RN: 553-26-4 MP (°C): 69

MW: 156.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.887E-02	4.509E+00	25	B095	2 0 1 1 2	

2015. C₁₀H₈N₂

α,α'-Dipyridyl

2,2'-Dipyridyl

α,α'-Bipyridyl

2,2'-Bipyridine

2,2'-Bipyridyl

RN: 366-18-7 MP (°C): 71.5

MW: 156.19 BP (°C): 273

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.201E-02	5.000E+00	20	F300	1 0 0 0 0	
4.276E-02	6.678E+00	24.99	B444	0 0 0 0 0	
3.778E-02	5.900E+00	25	B095	2 0 1 1 2	
4.094E-02	6.394E+00	25	K063	2 2 0 1 2	

2016. C₁₀H₈N₂O₂

4-Phenyluracil

4-Phenyl-uracil

RN: 21321-07-3 **MP (°C):**
MW: 188.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.314E-02	1.000E+01	100	F300	1 0 0 0 0	

2017. C₁₀H₈O

1-Naphthol

α-Naphthol

RN: 90-15-3 **MP (°C):** 96
MW: 144.17 **BP (°C):** 288

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.030E-03	8.694E-01	11	K307	2 0 1 2 2	
7.700E-03	1.110E+00	20	K130	2 1 1 1 2	
7.700E-03	1.110E+00	20	K301	2 2 1 1 1	
7.700E-03	1.110E+00	20	K307	2 0 1 2 2	
6.001E-03	8.653E-01	24	H106	1 0 2 2 2	
6.007E-03	8.660E-01	24	M303	1 0 1 1 2	
3.029E-03	4.367E-01	25	L085	1 2 0 1 2	
9.430E-03	1.360E+00	30	K307	2 0 1 2 2	
1.490E-02	2.148E+00	40	K307	2 0 1 2 2	
2.150E-02	3.100E+00	50	K307	2 0 1 2 2	

2018. C₁₀H₈O

2-Naphthol

β-Naphthol

RN: 135-19-3 **MP (°C):** 121
MW: 144.17 **BP (°C):** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.462E-03	3.550E-01	6.90	M026	2 0 1 2 2	
3.378E-03	4.870E-01	13.45	M026	2 0 1 2 2	
3.473E-03	5.007E-01	15.60	M027	1 0 0 2 2	
3.646E-03	5.257E-01	16.20	M027	1 0 0 2 2	
3.891E-03	5.610E-01	17.70	M026	2 0 1 2 2	
4.450E-03	6.416E-01	20	K130	2 1 1 1 2	
4.500E-03	6.488E-01	20	K301	2 2 1 1 1	
4.450E-03	6.416E-01	20	K308	1 0 0 1 2	
5.800E-03	8.362E-01	20	M122	2 0 2 2 2	
4.945E-03	7.130E-01	21.50	M026	2 0 1 2 2	
4.713E-03	6.795E-01	23.20	M027	1 0 0 2 2	
3.954E-03	5.700E-01	25	F300	1 0 0 0 2	

(continued)

2018. C₁₀H₈O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.240E-03	7.555E-01	25	K040	1 0 2 1 2	
5.356E-03	7.722E-01	25	L085	1 2 0 1 2	
6.929E-03	9.990E-01	25	R041	0 0 0 0 0	
6.076E-03	8.760E-01	29.50	M026	2 0 1 2 2	
6.431E-03	9.271E-01	31.30	M027	1 0 0 2 2	
6.832E-03	9.850E-01	33.30	M026	2 0 1 2 2	
9.045E-03	1.304E+00	38.70	M026	2 0 1 2 2	
1.116E-02	1.609E+00	44.50	M026	2 0 1 2 2	
1.388E-02	2.001E+00	49.50	M026	2 0 1 2 2	
1.706E-02	2.460E+00	55.20	M026	2 0 1 2 2	
2.104E-02	3.034E+00	60.00	M026	2 0 1 2 2	
2.928E-02	4.222E+00	68.10	M026	2 0 1 2 2	
3.810E-02	5.493E+00	75.00	M026	2 0 1 2 2	
4.670E-02	6.733E+00	80	K308	1 0 0 1 2	
5.129E-03	7.394E-01	ns	R427	0 0 0 0 0	

2019. C₁₀H₈O₂

2,3-Dihydroxynaphthalene

2,3-Dihydroxy-naphthalin

RN: 92-44-4 MP (°C): 162

MW: 160.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.830E-03	2.931E-01	20	M122	2 0 2 2 2	

2020. C₁₀H₈O₂

2,6-Dihydroxynaphthalene

2,6-Dihydroxy-naphthalin

RN: 581-43-1 MP (°C):

MW: 160.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-03	1.000E+00	14	F300	1 0 0 0 0	

2021. C₁₀H₉ClN₄O₂S

2-Sulfanilamido-5-chloropyrimidine

Benzenesulfonamide, 4-amino-N-(5-chloro-2-pyrimidinyl)-

RN: 4482-46-6 MP (°C):

MW: 284.73 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.322E-05	1.800E-02	37	R046	1 2 1 1 1	

2022. C₁₀H₉CIN₄O₂S

5-Sulfanilamido-2-chloropyrimidine

Benzenesulfonamide, 4-amino-N-(2-chloro-5-pyrimidinyl)-

RN: 17103-49-0 MP (°C):

MW: 284.73 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.127E-03	3.210E-01	37	R046	1 2 1 1 1	

2023. C₁₀H₉Cl₂NO

Acrylanilide, 3',4'-dichloro-2-methyl-Dicryl

RN: 2164-09-2 MP (°C): 127–128

MW: 230.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.477E-05	8.000E-03	ns	B185	0 0 0 0 0	

2024. C₁₀H₉Cl₃O₃

2,4,5-Trichlorophenoxy-γ-butyric acid

2,4,5-TB

4-(2,4,5-Trichlorophenoxy)butyric acid

4-(2,4,5-TB)

RN: 93-80-1 MP (°C): 114.5

MW: 283.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-04	4.200E-02	25	B164	1 0 1 1 1	
1.481E-04	4.200E-02	ns	B185	0 0 0 0 0	

2025. C₁₀H₉Cl₃O₃

2,4-Dichlorophenoxyacetic acid β-monochloroethyl ester

Ethanol, 2-chloro-, (2,4-dichlorophenoxy)acetate

RN: 19810-30-1 MP (°C):

MW: 283.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.910E-04	5.415E-02	ns	M120	0 0 1 1 2	

2026. C₁₀H₉Cl₄NO₂S

Captafol

cis-3α,4,7,7α-Tetrahydro-2-(1,1,2,2-tetrachloroethyl)thio-1H-isoindole-1,3(2H)-dione

Crisfolatan

Difolatan

Folcid

RN: 2939-80-2 **MP (°C):** 160.5**MW:** 349.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-06	1.422E-03	20	B179	0 0 0 0 0	
4.011E-06	1.400E-03	ns	M161	0 0 0 0 1	

2027. C₁₀H₉Cl₄O₄P

Gardona

2-Chloro-1-(2,4,5-trichlorophenyl)vinyldimethylphosphate

RN: 22248-79-9 **MP (°C):** 97.5**MW:** 365.97 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-05	1.100E-02	20	M061	1 0 0 0 1	

2028. C₁₀H₉Cl₄O₄P

Tetrachlorvinphos

2-Chloro-1-(2,4,5-trichlorophenyl)vinyl dimethyl phosphate

Rabon

Gardona

SD 8447

Stirofos

RN: 961-11-5 **MP (°C):** 96**MW:** 365.97 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-05	1.100E-02	20	M161	1 0 0 0 1	

2029. C₁₀H₉N

3-Methyl-isoquinoline

Isoquinoline, 3-methyl-

RN: 1125-80-0 **MP (°C):****MW:** 143.19 **BP (°C):** 519.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.418E-03	9.190E-01	20	A050	1 0 1 1 2	

2030. C₁₀H₉N

2-Naphthylamine

Naphthylamine-(2)

 β -Naphthylamin β -Naphthylamine

RN: 91-59-8

MP (°C): 113

MW: 143.19

BP (°C): 306.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.320E-03	1.890E-01	rt	N015	0 0 2 2 2	

2031. C₁₀H₉N

1-Naphthylamine

1-Aminonaphthalene

 α -Naphthoylamine α -Naphthylamin α -Naphthylamine

RN: 134-32-7

MP (°C): 50

MW: 143.19

BP (°C): 300.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.187E-02	1.700E+00	20	F300	1 0 0 0 1	
3.600E-04	5.155E-02	ns	L060	0 0 0 0 1	average

2032. C₁₀H₉NO

8-Hydroxyquinaldine

2-Methyl 8-quinolinol

RN: 826-81-3

MP (°C): 72.5

MW: 159.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E+03	3.916E+05	25.2	P024	2 2 1 1 2	
2.670E+03	4.250E+05	30.3	P024	2 2 1 1 2	

2033. C₁₀H₉NO

4-Hydroxy-2-methylquinoline

4-Hydroxy-2-methyl-chinolin

RN: 607-67-0

MP (°C): 234

MW: 159.19

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.282E-02	1.000E+01	20	F300	1 0 0 0 1	
5.936E-01	9.450E+01	100	F300	1 0 0 0 2	

2034. C₁₀H₉NO₂SEthyl *m*-isothiocyanobenzoate

Ethyl 3-isothiocyanobenzoate

RN: 3137-84-6 **MP (°C):****MW:** 207.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-04	5.181E-02	25	K032	2 2 0 1 2	

2035. C₁₀H₉NO₂S

Ethyl 4-isothiocyanatobenzoate

4-Carbethoxyphenylisothiocyanate

Ethyl *p*-isothiocyanatobenzoate**RN:** 1205-06-7 **MP (°C):****MW:** 207.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	1.865E-02	25	D019	1 1 1 1 1	

2036. C₁₀H₉NO₃S

Badische acid

2-Naphthylamine-8-sulfonic acid

Naphthylamin-(2)-sulfosaeure-(8)

RN: 86-60-2 **MP (°C):****MW:** 223.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.688E-03	6.000E-01	20	F300	1 0 0 0 2	

2037. C₁₀H₉NO₃S

2-Naphthylamine-1-sulfonic acid

α-Naphthylamine-*o*-monosulfonic acid**RN:** 81-16-3 **MP (°C):****MW:** 223.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-02	2.394E+00	0	D077	1 0 0 1 1	
1.429E-02	3.190E+00	10	D077	1 0 0 1 1	
1.829E-02	4.083E+00	20	D077	1 0 0 1 1	
2.317E-02	5.173E+00	30	D077	1 0 0 1 1	
2.893E-02	6.458E+00	40	D077	1 0 0 1 1	
3.555E-02	7.937E+00	50	D077	1 0 0 1 1	
4.435E-02	9.901E+00	60	D077	1 0 0 1 2	
6.010E-02	1.342E+01	70	D077	1 0 0 1 2	
7.834E-02	1.749E+01	80	D077	1 0 0 1 2	
1.028E-01	2.296E+01	90	D077	1 0 0 1 2	
1.347E-01	3.007E+01	100	D077	1 0 0 1 2	

2038. C₁₀H₉NO₃S

1-Naphthylamine-8-sulfonic acid

Naphthylamin-(1)-sulfosaeure-(8)

Peri acid

RN: 82-75-7 MP (°C):

MW: 223.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.958E-04	2.000E-01	21	F300	1 0 0 0 0	
1.971E-02	4.400E+00	100	F300	1 0 0 0 1	

2039. C₁₀H₉NO₃S

1-Naphthylamine-5-sulfonic acid

Laurent's acid

Naphthylamin-(1)-sulfosaeure-(5)

RN: 84-89-9 MP (°C):

MW: 223.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-03	1.000E+00	20	F300	1 0 0 0 2	

2040. C₁₀H₉NO₃S

1-Naphthylamine-4-sulfonic acid

4-Amino-1-naphthalenesulfonic acid

Naphthionic acid

Naphthylamin-(1)-sulfosaeure-(4)

Pirias acid

RN: 84-86-6 MP (°C): 000

MW: 223.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.209E-03	2.699E-01	0	D077	1 0 0 1 1	
1.299E-03	2.899E-01	10	D077	1 0 0 1 1	
1.388E-03	3.099E-01	20	D077	1 0 0 1 1	
1.344E-03	3.000E-01	20	F300	1 0 0 0 0	
1.657E-03	3.699E-01	30	D077	1 0 0 1 1	
2.149E-03	4.798E-01	40	D077	1 0 0 1 1	
2.641E-03	5.897E-01	50	D077	1 0 0 1 1	
3.357E-03	7.494E-01	60	D077	1 0 0 1 1	
4.341E-03	9.691E-01	70	D077	1 0 0 1 1	
5.815E-03	1.298E+00	80	D077	1 0 0 1 2	
7.825E-03	1.747E+00	90	D077	1 0 0 1 2	
1.021E-03	2.279E-01	100	D077	1 0 0 1 2	
1.075E-02	2.400E+00	100	F300	1 0 0 0 1	

2041. C₁₀H₉NO₃S

1,6-Cleve's acid

1-Naphthylamine-6-sulfonic acid

Naphthylamin-(1)-sulfosaeure-(6)

RN: 119-79-9 **MP (°C):****MW:** 223.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-03	1.000E+00	16	F300	1 0 0 0 2	

2042. C₁₀H₉NO₃S

Cassella's acid F

2-Naphthylamine-7-sulfonic acid

Naphthylamin-(2)-sulfosaeure-(7)

RN: 494-44-0 **MP (°C):****MW:** 223.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.958E-04	2.000E-01	20	F300	1 0 0 0 1	
1.389E-02	3.100E+00	100	F300	1 0 0 0 1	

2043. C₁₀H₉NO₃S

Bronner's acid

2-Naphthylamine-6-sulfonic acid

Naphthylamin-(2)-sulfosaeure-(6)

RN: 93-00-5 **MP (°C):****MW:** 223.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.375E-04	1.200E-01	20	F300	1 0 0 0 1	
7.615E-03	1.700E+00	100	F300	1 0 0 0 1	

2044. C₁₀H₉NO₃S

1-Naphthylamine-2-sulfonic acid

Naphthylamin-(1)-sulfosaeure-(2)

RN: 81-06-1 **MP (°C):****MW:** 223.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.836E-02	4.100E+00	20	F300	1 0 0 0 1	
1.402E-01	3.130E+01	100	F300	1 0 0 0 2	

2045. C₁₀H₉NO₃S

2-Naphthylamine-5-sulfonic acid

Dahl's acid

Naphthylamin-(2)-sulfosaeure-(5)

RN: 81-05-0 MP (°C):

MW: 223.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-03	3.300E-01	20	F300	1 0 0 0 2	

2046. C₁₀H₉NO₄S

7-Amino-1-naphthol-3-sulfonic acid

7-Amino-naphtol-(1)-sulfosaeure-(3)

RN: 90-51-7 MP (°C):

MW: 239.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.881E-02	4.500E+00	h	F300	0 0 0 0 1	

2047. C₁₀H₉NO₉S₃

1-Naphthylamine-2,4,7-trisulfonic acid

1,3,6-Naphthalenetrisulfonic acid, 4-amino-

RN: 61986-93-4 MP (°C):

MW: 383.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.799E-01	1.840E+02	20	F054	1 2 1 1 2	
8.216E-01	3.150E+02	80	F054	1 2 1 1 2	

2048. C₁₀H₉N₃O₃S

1-Sulfanilyl-3-methyl-5-pyrazolone

RN: MP (°C):

MW: 251.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.827E-03	4.590E-01	37	R045	1 2 1 1 2	

2049. C₁₀H₉N₄O₅

Picrolonic acid

Pikrolonsaeure

RN: 550-74-3

MP (°C): 116

MW: 265.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.394E-02	9.000E+00	17	F300	1 0 0 0 0	
3.582E-02	9.500E+00	100	F300	1 0 0 0 1	

2050. C₁₀H₁₀Fe

Ferrocene

bis-Cyclopentadienyliron

Ferrotsen

Iron bis(cyclopentadiene)

RN: 102-54-5

MP (°C):

MW: 186.04

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.388E-05	6.304E-03	25	B335	1 2 0 0 1	

2051. C₁₀H₁₀BrNO₃S4-Thiazolidinecarboxylic acid, 2-(5-bromo-2-hydroxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(5-bromo-2-hydroxyphenyl)-

RN: 256235-53-7 MP (°C):

MW: 304.17 BP (°C): 451.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.650E-01	21	B414	1 0 0 1 1	fast decomposition

2052. C₁₀H₁₀BrNO₄5-Bromo-2-*p*-phenyl-5-nitro-1,3-dioxane*m*-Dioxane, 5-bromo-5-nitro-2-phenyl-

1,3-Dioxane, 5-bromo-5-nitro-2-phenyl-

RN: 58522-87-5 MP (°C): 82-84

MW: 288.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.596E-03	4.598E-01	25	L013	1 0 2 1 2	

2053. C₁₀H₁₀BrNO₅5-Bromo-2-*p*-phenol-5-nitro-1,3-dioxane*m*-Dioxane, 5-bromo-5-nitro-2-phenol-

RN: 60766-61-2 MP (°C): 142–144

MW: 304.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-03	4.298E-01	25	L013	1 0 2 1 2	

2054. C₁₀H₁₀CINO₂S

4-Thiazolidinecarboxylic acid, 2-(4-chlorophenyl)-

4-Thiazolidinecarboxylic acid, 2-(*p*-chlorophenyl)-

Thiazolidine-4-carboxylic acid, (2-(4-chlorophenyl)-

RN: 34491-29-7 MP (C): 156–185 (°decomp)

MW: 243.71 BP (°C): 458.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-03	1.438E+00	21	B414	1 0 0 1 1	fast decomposition

2055. C₁₀H₁₀CINO₂S

4-Thiazolidinecarboxylic acid, 2-(2-chlorophenyl)-

4-Thiazolidinecarboxylic acid, 2-(*o*-chlorophenyl)-

Thiazolidine-4-carboxylic acid, 2-(2-chlorophenyl)-

RN: 72678-81-0 MP (°C): 145–147

MW: 243.71 BP (°C): 439.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	5.118E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2056. C₁₀H₁₀CINO₃

Chloroacetyl acetaminophen

Acetic acid, chloro-, 4-(acetylamino)phenyl ester

Acetanilide, 4'-hydroxy-, chloroacetate (ester)

RN: 17321-63-0 MP (°C): 184.5–185

MW: 227.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-03	2.800E-01	37	D029	0 0 0 0 0	

2057. C₁₀H₁₀Cl₂F₂N₂OS

3-[3-Chloro-4-(chlorodifluoromethylthio)phenyl]-1,1-dimethylurea
N-[3-Chloro-4-(chlorodifluoromethylthiol)phenyl]-*N,N'*-dimethylurea
N-(3-Chloro-4-difluorochloromethylthiophenyl)-*N,N'*-dimethylurea

Thiocchlormethyl

N-[3-Chloro-4-(chlorodifluoromethylthio)phenyl]-*N,N'*-dimethylurea

RN: 33439-45-1 **MP (°C):** 113.5

MW: 315.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.159E-01	6.803E+01	20	M161	1 0 0 0 1	

2058. C₁₀H₁₀Cl₂O₂

Chlorfenprop-methyl

Methyl 2-chloro-3-(*p*-chlorophenyl)propionate

Methyl α -*p*-dichlorohydrocinnamate

Bidisin

Fatex

RN: 14437-17-3 **MP (°C):**

MW: 233.10 **BP (°C):** 111.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.716E-04	4.000E-02	20	M161	1 0 0 0 1	

2059. C₁₀H₁₀Cl₂O₃

4-(2,4-Dichlorophenoxy)propionic acid

2,4-DB

RN: 94-82-6 **MP (°C):** 118

MW: 249.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	6.700E-02	25	B164	1 0 1 1 1	
1.847E-04	4.600E-02	25	M161	1 0 0 0 1	
2.128E-04	5.300E-02	ns	B185	0 0 0 0 0	
1.847E-04	4.600E-02	ns	L024	1 0 0 0 1	
2.128E-04	5.300E-02	rt	M061	0 0 0 0 1	

2060. C₁₀H₁₀Cl₂O₃

Ethyl (2,4-dichlorophenoxy)acetate

2,4-Dichlorophenoxyacetic acid ethyl ester

RN: 533-23-3 **MP (°C):**

MW: 249.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.529E-04	6.300E-02	ns	M120	0 0 1 1 2	

2061. C₁₀H₁₀Cl₈

Toxaphene

Camphechlor

Campheclor

PhenAcide

Toxakil

Chlorinated champhe

RN: 8001-35-2 **MP (°C):** 65**MW:** 413.82 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.329E-06	5.500E-04	20	M336	2 0 2 2 2	
9.666E-07	4.000E-04	25	C100	1 0 2 1 0	
1.208E-06	5.000E-04	25	P085	0 0 0 0 0	
1.788E-06	7.400E-04	25	W025	1 0 2 2 2	
1.450E-06	6.000E-04	ns	M110	0 0 0 0 0	EFG
1.329E-06	5.500E-04	ns	V414	0 0 0 0 0	
7.250E-06	3.000E-03	rt	M161	0 0 0 0 0	

2062. C₁₀H₁₀N₂O₄S

4-Thiazolidinecarboxylic acid, 2-(3-nitrophenyl)-

4-Thiazolidinecarboxylic acid, 2-(*m*-nitrophenyl)-**RN:** 69570-81-6 **MP (°C):** 151–153**MW:** 254.27 **BP (°C):** 500.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-03	1.348E+00	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2063. C₁₀H₁₀N₄O

Metamiton

3-Methyl-4-amino-6-phenyl-1,2,4-triazin-5(4H)-one

4-Amino-3-methyl-6-phenyl-1,2,4-triazin-5-one

Goltix

RN: 41394-05-2 **MP (°C):** 166.6**MW:** 202.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.901E-03	1.800E+00	20	M161	1 0 0 0 1	

2064. C₁₀H₁₀N₄O₂S

Sulfadiazine

Sulphadiazine

N1-(2-Pyrimidinyl)-sulfanilamide

Debenal

RN: 68-35-9**MP (°C):** 254**MW:** 250.28**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-04	5.907E-02	20	C006	1 2 1 1 2	
1.814E-04	4.540E-02	20	E003	2 2 1 1 2	
5.993E-04	1.500E-01	20	F073	1 2 2 2 2	
2.917E-04	7.299E-02	20	L058	1 0 1 1 1	
3.077E-04	7.700E-02	25	C102	2 0 2 2 2	
2.637E-03	6.600E-01	25	K048	1 2 2 1 1	pH 1.26
2.682E-04	6.713E-02	25	M440	0 0 0 0 0	
3.036E-04	7.599E-02	30	E003	2 2 1 1 2	
3.640E-04	9.110E-02	30	H018	0 0 0 0 0	
3.200E-04	8.009E-02	30	L069	1 0 1 1 0	EFG
7.192E-04	1.800E-01	35	H114	1 0 0 0 1	
5.074E-04	1.270E-01	37	C102	2 0 2 2 2	
4.914E-04	1.230E-01	37	F072	1 0 0 0 2	
4.794E-04	1.200E-01	37	F075	1 0 2 2 2	
5.114E-04	1.280E-01	37	K091	1 0 0 0 2	
5.194E-04	1.300E-01	37	L091	1 0 0 0 1	pH 5.5
7.192E-04	1.800E-01	37	M057	1 0 0 0 2	pH 5.5
8.790E-04	2.200E-01	37	R044	0 0 0 0 0	EFG, intrinsic
4.914E-04	1.230E-01	37	R045	1 2 1 1 1	
6.712E-04	1.680E-01	37	S192	1 0 1 1 2	pH 6.0
5.074E-04	1.270E-01	37	W016	2 0 1 1 2	
4.914E-04	1.230E-01	37	W053	1 0 0 0 2	
3.956E-04	9.900E-02	38	K006	1 0 0 0 1	
5.154E-04	1.290E-01	40	E003	2 2 1 1 2	
5.194E-04	1.300E-01	ns	G083	0 0 0 0 1	pH 5.5
3.196E-04	8.000E-02	ns	K444	0 0 0 0 0	
3.981E-04	9.964E-02	ns	R427	0 0 0 0 0	

2065. C₁₀H₁₀N₄O₂S

Sulfapyrazine

Sulphapyrazine

RN: 116-44-9**MP (°C):** 255**MW:** 250.28**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-04	5.000E-02	37	L091	1 0 0 0 0	pH 5.5

2066. C₁₀H₁₀N₄O₂S

5-Sulfanilamidopyrimidine

5-Sulfapyrimidine

Sulfanilamide, *N*1-5-pyrimidinyl-

RN: 17103-48-9 MP (°C):

MW: 250.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.916E-04	9.800E-02	37	R046	1 2 1 1 1	

2067. C₁₀H₁₀N₄O₂S

4-Sulfanilamidopyrimidine

4-Sulfapyrimidine

Sulfanilamide, *N*1-4-pyrimidinyl-

RN: 599-82-6 MP (°C):

MW: 250.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.414E-02	3.540E+00	37	R045	1 2 1 1 2	

2068. C₁₀H₁₀N₄O₄S

5-Sulfanilamidouracil

Benzenesulfonamide, 4-amino-*N*-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)-

RN: 6912-98-7 MP (°C):

MW: 282.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.722E-03	4.860E-01	37	R045	1 2 1 1 0	

2069. C₁₀H₁₀O

Benzalacetone

4-Phenyl-3-buten-2-one

Methyl styryl ketone

RN: 122-57-6 MP (°C):

MW: 146.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.560E-03	1.398E+00	25	R070	0 0 0 0 0	

2070. C₁₀H₁₀O₂*p*-Acetylacetophenone

Ethanone, 1,1'-(1,4-phenylene)bis-

RN: 1009-61-6 MP (°C):

MW: 162.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.890E-05	6.309E-03	25	C316	0 0 0 0 0	0.1M NaCl

2071. C₁₀H₁₀O₂

Methyl cinnamate

2-Propenoic acid

3-Phenyl-, methyl ester

RN: 103-26-4 MP (°C):

MW: 162.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	4.055E-01	25	R070	0 0 0 0 0	

2072. C₁₀H₁₀O₂*trans*- α -Methyl-cinnamic acid α -Methyl-*trans*-zimtsaeure

RN: 1895-97-2 MP (°C):

MW: 162.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.399E-03	1.200E+00	h	F300	0 0 0 0 1	

2073. C₁₀H₁₀O₄Dimethyl *o*-phthalate

RN: MP (°C): 5.5 C

MW: 194.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.802E-02	3.500E+00	25	S417	0 0 0 0 0	

2074. C₁₀H₁₀O₄

Ferulic acid

3-(4-Hydroxy-3-methoxyphenyl)-2-propenoic acid

4-Hydroxy-3-methoxycinnamic acid

RN: 1135-24-6 **MP (°C):** 169 C**MW:** 194.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.935E-03	5.700E-01	15	M461	0 0 0 0 0	
4.017E-03	7.800E-01	25	M461	0 0 0 0 0	
4.738E-03	9.200E-01	30	M461	0 0 0 0 0	
9.063E-03	1.760E+00	40	M461	0 0 0 0 0	
1.128E-02	2.190E+00	50	M461	0 0 0 0 0	

2075. C₁₀H₁₀O₄Acetyl-*r*-mandelic acid(R)(-)*O*-Acetylmandelic acid[R]-[-]- α -(Acetoxy)phenylacetic acid*O*-Acetylmandelic acid**RN:** 5438-68-6 **MP (°C):****MW:** 194.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.919E-02	5.668E+00	0	A043	1 2 1 1 1	
2.919E-02	5.668E+00	0	L035	1 2 2 1 1	
3.478E-02	6.754E+00	10	A043	1 2 1 1 1	
3.478E-02	6.754E+00	10	L035	1 2 2 1 1	
3.884E-02	7.543E+00	15	A043	1 2 1 1 1	
3.884E-02	7.543E+00	15	L035	1 2 2 1 1	
4.897E-02	9.509E+00	20	A043	1 2 1 1 1	
4.897E-02	9.509E+00	20	L035	1 2 2 1 1	
5.804E-02	1.127E+01	25	A043	1 2 1 1 2	
5.804E-02	1.127E+01	25	L035	1 2 2 1 2	
7.060E-02	1.371E+01	30	A043	1 2 1 1 2	
7.060E-02	1.371E+01	30	L035	1 2 2 1 2	
1.005E-01	1.951E+01	35	A043	1 2 1 1 2	
1.587E-01	3.082E+01	40	A043	1 2 1 1 2	
2.795E-01	5.428E+01	45	A043	1 2 1 1 2	
2.795E-01	5.428E+01	45	L035	1 2 2 1 2	
6.125E-01	1.189E+02	50	A043	1 2 1 1 2	
6.125E-01	1.189E+02	50	L035	1 2 2 1 2	

2076. C₁₀H₁₀O₄

Dimethyl phthalate

1,2-Benzenedicarboxylic acid, dimethyl ester

Fermine

Unimoll DM

Mipax

Palatinol M

RN: 131-11-3 **MP (°C):** 5.5
MW: 194.19 **BP (°C):** 283.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E-02	4.292E+00	20	L300	2 1 0 2 2	
4.087E-02	7.937E+00	20.00	D343	0 0 0 0 0	
2.317E-01	4.500E+01	25	F067	1 0 2 2 2	<i>sic</i>
2.307E-02	4.480E+00	c	F070	1 0 0 0 0	
1.566E-02	3.041E+00	ns	F014	0 0 0 0 2	
2.052E-02	3.984E+00	ns	H069	0 0 1 1 1	
2.214E-02	4.300E+00	rt	M161	0 0 0 0 1	

2077. C₁₀H₁₀O₄

Meconin

Mekonin

RN: 569-31-3 **MP (°C):** 102
MW: 194.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.287E-02	2.500E+00	25	F300	1 0 0 0 0	
2.420E-02	4.700E+00	100	F300	1 0 0 0 1	

2078. C₁₀H₁₀O₄

Acetylsalicylic acid, methyl ester

Methyl 2-acetoxybenzoate

Benzoic acid, 2-(acetoxy)-, methyl ester

RN: 580-02-9 **MP (°C):** 48
MW: 194.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-02	2.810E+00	21	N335	0 0 0 0 0	
1.679E-02	3.260E+00	37	G430	0 0 0 0 0	pH 4.5

2079. C₁₀H₁₀O₄

Terephthalate acid dimethyl ester
 Terephthalsaeure-dimethyl ester
 1,4-Benzenedicarboxylic acid dimethyl ester
 Terephthalic acid
 Dimethyl terephthalate
 Dimethyl 1,4-Benzenedicarboxylate
RN: 120-61-6 **MP (°C):** 140
MW: 194.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E-04	3.282E-02	25	C316	0 0 0 0 0	0.1M NaCl
1.540E-02	2.991E+00	h	F070	1 0 0 0 1	

2080. C₁₀H₁₀O₅

Opianic acid
 Opiansaeure
RN: 519-05-1 **MP (°C):** 150
MW: 210.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.189E-02	2.500E+00	20	F300	1 0 0 0 1	
8.088E-02	1.700E+01	h	F300	0 0 0 0 1	

2081. C₁₀H₁₁ClO₃

Mecoprop
 2-(4-Chloro-2-methylphenoxy)propionic acid
 2-(2-Methyl-4-chlorophenoxy)propionic acid
 2-(MCPP)
RN: 93-65-2 **MP (°C):** 93
MW: 214.65 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-03	6.200E-01	20	B185	0 0 0 0 0	
2.795E-03	6.000E-01	20	B200	1 0 0 0 2	
2.887E-03	6.196E-01	20	M061	1 0 0 0 1	
2.888E-03	6.200E-01	20	M161	1 0 0 0 2	
4.170E-03	8.950E-01	25	B164	1 0 1 1 2	
4.170E-03	8.950E-01	25	B185	0 0 0 0 0	
2.794E-03	5.996E-01	ns	B100	0 0 0 0 0	
2.050E-04	4.400E-02	ns	B185	0 0 0 0 0	
2.888E-03	6.200E-01	ns	L024	1 0 0 0 2	
3.802E-03	8.161E-01	ns	R427	0 0 0 0 0	

2082. C₁₀H₁₁ClO₃

4-(4-Chlorophenoxy)butyric acid

4-(4-CPB)

RN: 3547-07-7

MP (°C):

MW: 214.65

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.125E-04	1.100E-01	25	B164	1 0 1 1 2	

2083. C₁₀H₁₁Cl₃O₂

2,3,6-Trichlorobenzylxymethoxypropanol

1-Propanol, 3-[(2,3,6-trichlorobenzyl)oxy]-

RN: 1591-82-8

MP (°C):

MW: 269.56

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.708E-04	7.300E-02	25	B185	0 0 0 0 0	
2.708E-04	7.300E-02	25	B200	1 0 0 0 1	

2084. C₁₀H₁₁FN₂O₆

1,3-bis(Acetoxyethyl)-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

1,3-bis(Acetoxyethyl)-5-fluorouracil

RN: 66542-48-1

MP (°C): 105–106

MW: 274.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.568E-02	4.300E+00	22	B321	0 0 0 0 0	pH 4.0

2085. C₁₀H₁₁F₃N₂O

Fluometuron

1,1-Dimethyl-3-(α,α,α -trifluoro-*m*-tolyl)urea

RN: 2164-17-2

MP (°C): 163

MW: 232.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	1.061E-01	20	B179	0 0 0 0 0	
4.522E-04	1.050E-01	20	M161	1 0 0 0 2	
3.661E-04	8.500E-02	24	C105	2 1 2 2 2	
3.876E-04	9.000E-02	25	B200	1 0 0 0 1	
3.876E-04	9.000E-02	25	G036	1 0 0 0 1	
3.876E-04	9.000E-02	25	M061	1 0 0 0 1	

2086. C₁₀H₁₁F₃N₂O₃S

Fluoridamid

Acetamide, *N*-{4-methyl-3-{{(trifluoromethyl)sulfonyl}amino}phenyl}-

Sustar

MBR6033

RN: 47000-92-0 MP (°C): 182–184

MW: 296.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.388E-04	1.300E-01	22	G307	0 0 0 0 0	

2087. C₁₀H₁₁NO*N*-Methylcinnamide2-Propenamide, *N*-methyl-3-phenyl-

RN: 2757-10-0 MP (°C):

MW: 161.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.310E-02	2.112E+00	ns	H350	0 0 0 0 0	

2088. C₁₀H₁₁NOS*m*-Isopropoxyphenyl isothiocyanate

3-Isopropoxyphenyl isothiocyanate

RN: 3528-90-3 MP (°C):

MW: 193.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-04	9.084E-02	25	K032	2 2 0 1 2	

2089. C₁₀H₁₁NO₂S

2-Phenylthiazolidine-4-carboxylic acid

4-Thiazolidinecarboxylic acid, 2-phenyl-

RN: 42607-21-6 MP (°C): 166–168

MW: 209.27 BP (°C): 433.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-03	9.417E-01	21	B414	1 0 0 1 1	partial decomposition

2090. C₁₀H₁₁NO₃Acetamide, 2-(benzoyloxy)-*N*-methyl-

RN: 106231-50-9 MP (°C): 111

MW: 193.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.915E-02	3.700E+00	22	B427	1 0 0 1 1	
1.915E-02	3.700E+00	22	N317	1 1 2 1 2	in 0.01M HCl

2091. C₁₀H₁₁NO₃*p*-Acetoxy-acetanilide*p*-Acetoxyacetanilide

Acetaminophen acetate

Acetyl acetaminophen

RN: 2623-33-8 MP (°C): 153

MW: 193.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.656E-03	3.200E-01	25	B010	1 1 1 1 0	
1.237E-02	2.390E+00	25	E016	1 1 1 1 2	
1.139E-02	2.200E+00	25	M333	1 1 0 0 2	
1.760E-02	3.400E+00	37	D029	0 0 0 0 0	

2092. C₁₀H₁₁NO₃S

4-Thiazolidinecarboxylic acid, 2-(4-hydroxyphenyl)-

4-Thiazolidinecarboxylic acid, 2-(*p*-hydroxyphenyl)-

RN: 69588-11-0 MP (°C):

MW: 225.27 BP (°C): 507.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-03	1.577E+00	21	B414	1 0 0 1 1	fast decomposition

2093. C₁₀H₁₁NO₃S

2-(2-Hydroxyphenyl)-4-thiazolidinecarboxylic acid

4-Thiazolidinecarboxylic acid, 2-(2-hydroxyphenyl)-

Thiazolidine-4-carboxylic acid, 2-(2-hydroxyphenyl)

RN: 72678-82-1 MP (°C):

MW: 225.27 BP (°C): 418.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	4.731E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2094. C₁₀H₁₁NO₄

Methyl acetaminophen

Carbonic acid, 4-(acetylamino)phenyl methyl ester

Acetanilide, 4'-hydroxy-, methyl carbonate (ester)

RN: 17321-62-9 **MP (°C):** 115.5–116.5**MW:** 209.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.868E-02	6.000E+00	37	D029	0 0 0 0 0	

2095. C₁₀H₁₁NO₄*O*-(Acetoxymethyl) salicylamide

2-[(Acetoxy)methoxy]-benzamide

Benzamide, 2-[(acetoxy)methoxy]-

O-Acetoxyethyl methyl salicylamide**RN:** 102273-25-6 **MP (°C):** 92.5**MW:** 209.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.39E-02	>5.000E+00	23	B328	1 2 2 1 1	pH 4
2.390E-02	5.000E+00	23	B328	0 0 0 0 0	

2096. C₁₀H₁₁NO₄

Carbobenzoxyglycine

N-Carbobenzyloxyglycine*N*-CBZ-glycine

Benzoyloxycarbonyl glycine

RN: 1138-80-3 **MP (°C):****MW:** 209.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.180E-02	4.560E+00	25.1	N026	0 0 0 0 0	
2.170E-02	4.539E+00	25.1	N027	1 1 2 2 2	

2097. C₁₀H₁₁NO₅

Acido d-feniltartrammico tartranilico

RN: **MP (°C):** 194**MW:** 225.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.232E-01	2.774E+01	17.40	C070	1 2 2 1 2	

2098. C₁₀H₁₁NO₆Acido *p*-ossifeniltartrammico

RN: **MP (°C):** 218
MW: 241.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-01	4.045E+01	14	C071	1 2 0 1 2	

2099. C₁₀H₁₁N₃OS

Methabenztiazuron

N-2-Benzothiazolyl-*N,N'*-dimethylurea
 1,3-Dimethyl-3-(2-benzothiazolyl)urea
 Methyl-*N'*-methyl-*N'*-(2-benzothiazolyl)urea
 Tribunil
 Preparation 5633

RN: 18691-97-9 **MP (°C):** 119.5
MW: 221.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.666E-04	5.900E-02	20	M161	1 0 0 0 1	

2100. C₁₀H₁₁N₃O₂S₂

Methyl sulfathiazole

Sulfathiazol methyle

RN: 15251-46-4 **MP (°C):**
MW: 269.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.653E-04	2.600E-01	37	D084	1 0 1 0 1	

2101. C₁₀H₁₁N₃O₂S

Sulfapyrrole

RN: **MP (°C):**
MW: 237.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.023E-02	4.800E+00	20	F073	1 2 2 2 2	

2102. C₁₀H₁₁N₃O₂S₂

Sulfamethylthiazole

4-Methyl-2-sulfanilamidothiazole

2-(*p*-Aminobenzenesulfonamido)-4-methylthiazole

2-Sulfanilamido-4-methylthiazole

Aseptil 2

Ciba 3753

RN: 515-59-3 **MP (°C):** 239**MW:** 269.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.084E-04	1.100E-01	20	F073	1 2 2 2 2	
4.084E-04	1.100E-01	20	F074	1 0 0 0 2	

2103. C₁₀H₁₁N₃O₂S₂N1-Methyl-*N*1-2-thiazolyl-sulfanilamide

N1-Methylsulfathiazole

RN: 51203-19-1 **MP (°C):****MW:** 269.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-03	3.097E-01	37	K095	2 0 0 0 2	intrinsic

2104. C₁₀H₁₁N₃O₃α-Semicarbazono-*p*-tolyl acetate**RN:** **MP (°C):****MW:** 221.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-03	3.097E-01	25	A066	1 0 1 1 1	

2105. C₁₀H₁₁N₃O₃S

Sulfamethoxazole

4-Amino-*N*-(5-methyl-3-isoxazolyl)benzenesulfonamide

Cotrimoxazole

Septra

Bactrim

Cotrim

RN: 723-46-6 **MP (°C):** 167**MW:** 253.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.109E-03	2.810E-01	25	D308	0 0 0 0 0	pH 3.22
1.730E-03	4.383E-01	25	F415	0 0 0 0 0	Average

(continued)

2105. C₁₀H₁₁N₃O₃S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-03	3.723E-01	25	M440	0 0 0 0 0	
1.974E-03	5.000E-01	25	R025	0 0 0 0 0	
1.488E-03	3.770E-01	32	D308	0 0 0 0 0	pH 4.0
1.824E-03	4.620E-01	37	D308	0 0 0 0 0	pH 3.43
2.408E-03	6.100E-01	37	H120	1 1 1 1 1	normal saline
2.480E-03	6.281E-01	37	K095	2 0 0 0 2	intrinsic
5.527E-03	1.400E+00	37	M321	1 0 0 0 2	intrinsic
1.540E-03	3.900E-01	amb	L434	0 0 0 0 0	
1.540E-03	3.900E-01	amb	L437	0 0 0 0 0	
3.948E-05	1.000E-02	ns	K444	0 0 0 0 0	

2106. C₁₀H₁₁N₅O₂S

5-Sulfanilamido-2-aminopyrimidine

Benzenesulfonamide, 4-amino-N-(2-amino-5-pyrimidinyl)-

RN: 71119-38-5 MP (°C):

MW: 265.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.129E-04	8.300E-02	37	R046	1 2 1 1 1	

2107. C₁₀H₁₂

Tetralin

1,2,3,4-Tetrahydronaphthalene

RN: 119-64-2 MP (°C): -31.0

MW: 132.21 BP (°C): 207.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.404E-04	4.500E-02	20	B356	0 0 0 0 0	
3.532E-04	4.670E-02	28	B348	2 1 2 2 2	
1.513E-03	2.000E-01	150	J023	1 1 2 2 0	
3.026E-03	4.000E-01	200	J023	1 1 2 2 0	
3.026E-02	4.000E+00	250	J023	1 1 2 2 0	
3.236E-04	4.278E-02	ns	D001	0 0 0 0 2	

2108. C₁₀H₁₂BrCl₂O₃PS

Bromophos-ethyl

O-(4-Bromo-2,5-dichlorophenyl) *O,O*-diethyl phosphorothioate

Nexagan

Filariol

RN: 4824-78-6**MP (°C):****MW:** 394.06**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.329E-07	2.100E-04	10	B324	0 0 0 0 0	
5.329E-07	2.100E-04	10	B324	0 0 0 0 0	
8.629E-07	3.400E-04	20	B324	0 0 0 0 0	
8.628E-07	3.400E-04	20	B324	0 0 0 0 0	
7.613E-06	3.000E-03	20	F311	1 2 2 2 1	
5.075E-06	2.000E-03	20	W312	1 0 0 0 0	
1.269E-06	5.001E-04	30	B324	0 0 0 0 0	
1.269E-06	5.000E-04	30	B324	0 0 0 0 0	
5.075E-06	2.000E-03	ns	E050	0 0 0 0 0	
5.075E-06	2.000E-03	rt	M161	0 0 0 0 0	

2109. C₁₀H₁₂ClNO₂

Chloro-IPC

Furloe

Taterpex

Chlorpropham

Isopropyl *m*-chlorocarbanilate**RN:** 101-21-3**MP (°C):** 38**MW:** 213.67**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.055E-04	1.080E-01	20	B185	0 0 0 0 0	
3.744E-04	8.000E-02	25	G099	1 0 0 1 0	
3.744E-04	8.000E-02	25	G319	0 0 0 0 0	
4.165E-04	8.900E-02	25	M161	1 0 0 0 1	
3.744E-04	8.000E-02	ns	B185	0 0 0 0 0	
4.119E-04	8.800E-02	ns	B200	0 0 0 0 1	
3.744E-04	8.000E-02	ns	F035	0 0 0 0 0	
4.119E-04	8.800E-02	ns	H042	0 0 0 0 1	
3.744E-04	8.000E-02	ns	M061	0 0 0 0 1	
3.548E-04	7.581E-02	ns	M163	0 0 0 0 0	EFG
5.055E-04	1.080E-01	ns	N013	0 0 0 0 2	

2110. C₁₀H₁₂ClNO₂

Baclofen

Lioresal

 β -(Aminomethyl)-*p*-chlorohydrocinnamic acid**RN:** 1134-47-0 **MP (°C):****MW:** 213.67 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.129E-02	4.549E+00	25	M374	1 0 2 1 2	

2111. C₁₀H₁₂ClN₃O₂

Tranid

3-Chloro-6-cyanonorbornanone-2-oxime-*O,N*-methylcarbamate**RN:** 15271-41-7 **MP (°C):** 143.5**MW:** 241.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.259E-03	1.996E+00	ns	M061	0 0 0 0 0	

2112. C₁₀H₁₂ClN₃O₃S

Quinethazone

7-Chloro-2-ethyl-1,2,3,4-tetrahydro-4-oxo-6-quinazolinesulfonamide

Hydromox

CL 36010

Aquamox

RN: 73-49-4 **MP (°C):** 251**MW:** 289.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.176E-04	1.500E-01	25	A081	1 0 1 1 0	EFG

2113. C₁₀H₁₂ClN₅O₂

2-Chloro-2',3'-dideoxyadenosine

2-CIDDA

RN: 114849-58-0 **MP (°C):****MW:** 269.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.745E-03	1.010E+00	25	A336	0 0 0 0 0	

2114. C₁₀H₁₂Cl₂O

2,4-Dichloro-6-butyl-phenol

Phenol, 2-butyl-4,6-dichloro-

RN: 91399-13-2 MP (°C):

MW: 219.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.259E-02	25	B316	0 0 0 0 0	

2115. C₁₀H₁₂Cl₃O₂PS

Trichloronate

Trichloronat

Ethyl *O*-(2,4,5-trichlorophenyl) ethylphosphonothioate

Agritox

Bay 37289

RN: 327-98-0 MP (°C):

MW: 333.60 BP (°C): 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.458E-06	8.200E-04	10	B324	0 0 0 0 0	
2.458E-06	8.200E-04	10	B324	0 0 0 0 0	
1.769E-06	5.901E-04	20	B300	2 1 1 1 2	
2.638E-06	8.800E-04	20	B324	0 0 0 0 0	
2.638E-06	8.800E-04	20	B324	0 0 0 0 0	
1.499E-04	5.000E-02	20	M161	1 0 0 0 1	sic
3.208E-06	1.070E-03	30	B324	0 0 0 0 0	
3.207E-06	1.070E-03	30	B324	0 0 0 0 0	

2116. C₁₀H₁₂N₂O₂Acetone *N*-(phenylcarbamoyl)oximeAcetone oxime *N*-phenylcarbamate

Proxypham

RN: MP (°C): 109.5

MW: 192.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.601E-03	5.000E-01	ns	M061	0 0 0 0 2	approximate

2117. C₁₀H₁₂N₂O₃

Barbituric-2-14C acid, 5,5-diallyl

RN: 112599-90-3 MP (°C):

MW: 208.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.381E-03	1.745E+00	25	P350	0 0 0 0 0	intrinsic

2118. C₁₀H₁₂N₂O₃

Allobarbital

5,5-Diallylbarbituric acid

RN: 52-43-7

MP (°C): 171

MW: 208.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.003E-03	1.250E+00	20	J030	1 2 2 2 2	
7.193E-03	1.498E+00	25	A023	1 0 0 1 2	
8.500E-03	1.770E+00	25	G003	1 1 1 1 1	pH 4.7
8.650E-03	1.801E+00	25	V033	2 0 1 1 2	
8.700E-03	1.812E+00	25.00	T303	1 0 0 0 1	
9.250E-03	1.926E+00	30	G014	1 1 1 1 0	EFG
9.200E-03	1.916E+00	30	I001	2 0 2 1 0	EFG, 0.003N H ₂ SO ₄
9.200E-03	1.916E+00	30	K108	1 2 2 0 1	
1.150E-02	2.394E+00	35	A023	1 0 0 1 2	
1.110E-02	2.311E+00	35.00	T303	1 0 0 0 2	
1.215E-02	2.530E+00	37	J030	1 2 2 2 2	
1.200E-02	2.499E+00	37	K121	1 2 1 2 1	0.1N HCl
1.675E-02	3.488E+00	40	A023	1 0 0 1 2	
1.370E-01	2.853E+01	40	N008	1 0 1 1 2	sic
1.690E-02	3.519E+00	45.00	T303	1 0 0 0 2	
7.036E-03	1.465E+00	ns	T003	0 0 0 0 2	

2119. C₁₀H₁₂N₂O₃S

Bentazon

2,1,3-Benzothiadiazin-4(3H)-one

Thiadiazinol

Basagran 4E

Adagio

BAS 351H

RN: 25057-89-0 MP (°C): 138.0

MW: 240.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-03	5.000E-01	20	M161	1 0 0 0 2	
2.080E-03	4.998E-01	ns	B100	0 0 0 0 0	
3.329E-03	8.000E-01	ns	M110	0 0 0 0 0	EFG

2120. C₁₀H₁₂N₂O₄

Stavudine

1-(2,3-Dideoxy-β-D-glycero-pent-2-enofuranosyl)thymine

BMY-27857

d4T

Zerit

3'-Deoxy-2'-thymidinene

RN: 3056-17-5 **MP (°C):** 159–160**MW:** 224.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.353E-01	7.519E+01	20.5	M439	0 0 0 0 0	
3.791E-01	8.500E+01	24.8	M439	0 0 0 0 0	
4.238E-01	9.502E+01	29.4	M439	0 0 0 0 0	
4.668E-01	1.047E+02	33.2	M439	0 0 0 0 0	
5.563E-01	1.247E+02	38.4	M439	0 0 0 0 0	
3.702E-01	8.300E+01	ns	K444	0 0 0 0 0	
3.418E-01	7.664E+01	ns	S469	0 0 0 0 0	

2121. C₁₀H₁₂N₂O₄S

N1,N4-Diacetylsulfanilamide

N4-Acetyl sulphacetamide

RN: 5626-90-4 **MP (°C):****MW:** 256.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.389E-03	2.150E+00	37	L091	1 0 0 0 2	pH 5.5

2122. C₁₀H₁₂N₂O₅

D-Monofeniltartramide tartranilamide

RN: **MP (°C):** 226**MW:** 240.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-02	4.704E+00	21.50	C070	1 2 2 1 2	

2123. C₁₀H₁₂N₂O₅2,4-Dinitro-6-*sec*-butylphenol

Dinoseb

4,6-Dinitro-2-*S*-butylphenolPhenol, 4,6-dinitro-2-*sec*-butyl-

RN: 88-85-7 MP (°C): 38

MW: 240.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.165E-04	5.200E-02	25	B200	1 0 0 0 1	
2.165E-04	5.200E-02	25	G319	0 0 0 0 0	
3.053E-03	7.335E-01	25	M061	1 0 0 0 2	
4.159E-03	9.990E-01	ns	B100	0 0 0 0 0	
2.081E-04	5.000E-02	ns	B185	0 0 0 0 0	
1.413E-03	3.393E-01	ns	M163	0 0 0 0 0	EFG
2.165E-04	5.200E-02	ns	V414	0 0 0 0 0	
4.163E-04	1.000E-01	rt	M161	0 0 0 0 2	

2124. C₁₀H₁₂N₂O₅S

7-Aminocephalosporanic acid

7-ACA

RN: 957-68-6 MP (°C):

MW: 272.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.901E-04	2.696E-01	1.29	W417	0 0 0 0 0	
1.070E-03	2.914E-01	5.19	W417	0 0 0 0 0	
1.130E-03	3.076E-01	8.29	W417	0 0 0 0 0	
1.255E-03	3.416E-01	12.19	W417	0 0 0 0 0	
1.367E-03	3.723E-01	17.59	W417	0 0 0 0 0	
1.504E-03	4.096E-01	22.99	W417	0 0 0 0 0	
1.627E-03	4.429E-01	27.99	W417	0 0 0 0 0	

2125. C₁₀H₁₂N₃O₃PS₂

Azinphos-methyl

Guthion

S-(3,4-Dihydro-4-oxobenzo[d][1,2,3]triazin-3-ylmethyl) O,O-dimethyl phosphorodithioate

Methyl gusathion

RN: 86-50-0 MP (°C): 74

MW: 317.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.994E-05	9.501E-03	10	B324	0 0 0 0 0	
2.994E-05	9.500E-03	10	B324	0 0 0 0 0	
4.412E-05	1.400E-02	15	A087	1 0 0 1 0	
6.587E-05	2.090E-02	20	B300	2 1 1 1 2	

(continued)

2125. C₁₀H₁₂N₃O₃PS₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.587E-05	2.090E-02	20	B324	0 0 0 0 0	
6.586E-05	2.090E-02	20	B324	0 0 0 0 0	
9.454E-05	3.000E-02	20	M061	1 0 0 0 1	
9.139E-05	2.900E-02	25	A087	1 0 0 1 0	
1.374E-04	4.360E-02	30	B324	0 0 0 0 0	
1.374E-04	4.360E-02	30	B324	0 0 0 0 0	
1.481E-04	4.700E-02	35	A087	1 0 0 1 0	
8.913E-05	2.828E-02	ns	R427	0 0 0 0 0	
1.040E-04	3.300E-02	rt	M161	0 0 0 0 1	

2126. C₁₀H₁₂N₄

6,7-Diethylpteridine

RN: MP (°C): 52
MW: 188.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.641E-01	1.250E+02	20	A019	2 2 1 1 0	

2127. C₁₀H₁₂N₄O

2-Hydroxy-6,7-diethylpteridine
 2-Hydroxy-6:7-diethylpteridine
 4-Hydroxy-6,7-diethylpteridine
 4-Hydroxy-6:7-diethylpteridine

RN: 90870-76-1 MP (°C):
MW: 204.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.221E-02	2.494E+00	20	A019	2 2 1 1 2	
5.434E-03	1.110E+00	20	A019	2 2 1 1 2	

2128. C₁₀H₁₂N₄O₂

2,4-Dihydroxy-6,7-diethylpteridine
 2,4-Dihydroxy-6:7-diethylpteridine
RN: 113222-29-0 MP (°C): 218
MW: 220.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.124E-03	9.083E-01	20	A019	2 2 1 1 2	

2129. C₁₀H₁₂N₄O₂

1H-Pyrazolo[3,4-d]pyrimidine, 4-[(tetrahydro-2H-pyran-2-yl)oxy]-2-Tetrahydropuran-4-allopurinyl ether

RN: 52717-52-9 **MP (°C):**
MW: 220.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-02	3.640E+00	ns	H067	0 0 0 0 0	

2130. C₁₀H₁₂N₄O₂S

Sulfaethidole

Ethyl thiodiazole

Sulfaethylthiadiazole

Thiodiazolique ethyle

RN: 94-19-9 **MP (°C):** 188
MW: 252.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.522E-04	2.150E-01	20	F073	1 2 2 2 2	
1.288E-02	3.250E+00	37	B046	1 0 2 2 2	pH 5
1.585E-03	4.000E-01	37	D084	1 0 1 0 1	

2131. C₁₀H₁₂N₄O₃

1-Butyryloxymethyl allopurinol

Butanoic acid, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester

RN: 98827-21-5 **MP (°C):** 224–226
MW: 236.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.482E-03	3.500E-01	22	B322	0 0 0 0 0	

2132. C₁₀H₁₂N₄O₃

2',3'-Dideoxyinosine

Videx

Didanosine

CCRIS 805

CCRIS 805Didanosine

RN: 69655-05-6 **MP (°C):** 175
MW: 236.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.614E-02	1.090E+01	4	A337	0 0 0 0 0	
1.156E-01	2.730E+01	25	A337	0 0 0 0 0	
1.270E-01	3.000E+01	ns	A426	0 0 0 0 0	Intrinsic
1.156E-01	2.730E+01	ns	K444	0 0 0 0 0	
1.125E-01	2.657E+01	ns	S469	0 0 0 0 0	

2133. C₁₀H₁₂N₄O₃

2-Butyryloxymethyl allopurinol

Butanoic acid, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester

RN: 98827-22-6 MP (°C): 182–183

MW: 236.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.350E-03	1.500E+00	22	B322	0 0 0 0 0	

2134. C₁₀H₁₂N₄O₄

2'-Deoxy-inosine

2-[Deoxyinosine

Deoxyinosine

RN: 890-38-0 MP (°C):

MW: 252.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.301E-02	8.326E+00	25.02	T420	0 0 0 0 0	

2135. C₁₀H₁₂N₄O₅

Inosine

Inosin

Hypoxanthine ribonucleoside

RN: 58-63-9 MP (°C): 212dec

MW: 268.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.871E-02	1.575E+01	20	D041	1 0 0 0 1	
5.890E-02	1.580E+01	20	F300	1 0 0 0 2	
5.888E-02	1.579E+01	ns	R427	0 0 0 0 0	

2136. C₁₀H₁₂N₄O₆

2,4,6-Trinitrodiethylaniline

2-4-6-Trinitrodiethylaniline

RN: 106415-21-8 MP (°C):

MW: 284.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.759E-04	5.000E-02	50	D067	1 2 0 0 0	
7.037E-04	2.000E-01	100	D067	1 2 0 0 1	

2137. C₁₀H₁₂N₅O₆P

Adenosine 3':5'-monophosphate

Adenosine, cyclic 3',5'-(hydrogen phosphate)

4H-Furo[3,2-d]-1,3,2-dioxaphosphorin, adenosine deriv

RN: 60-92-4 MP (°C):

MW: 329.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.360E-02	7.769E+00	20	D034	0 0 0 0 0	pH 7.0

2138. C₁₀H₁₂N₆O₂S

2-S-Cysteinyl-4,6-bis-(dimethylamino)-s-triazine

RN: MP (°C): 173

MW: 280.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.991E-03	2.240E+00	25	C051	1 2 1 1 2	pH 7

2139. C₁₀H₁₂O

Estragole

1-Methoxy-4-(2-propen-1-yl)benzene

Chavicyl methyl ether

4-Allylanisole

Tarragon

RN: 140-67-0 MP (°C): <25

MW: 148.21 BP (°C): 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	1.778E-01	25	I019	1 0 1 2 2	

2140. C₁₀H₁₂O

Anethole

Methoxy-4-propenylbenzene

Propenylanisole

p-Propenylanisole

Anise camphor

Isoestragole

RN: 104-46-1 MP (°C): 21.4

MW: 148.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.482E-01	25	D407	1 0 2 2 2	
7.490E-04	1.110E-01	25	I019	1 0 1 2 2	
7.413E-04	1.099E-01	ns	S460	0 0 0 0 0	

2141. C₁₀H₁₂O

5,6,7,8-Tetrahydro-2-naphthol

5,6,7,8-Tetrahydro-naphthol-(2)

RN: 1125-78-6 **MP (°C):** 56.5
MW: 148.21 **BP (°C):** 275.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.012E-02	1.500E+00	20	F300	1 0 0 0 1	

2142. C₁₀H₁₂O₂

Eugenol

1-Allyl-3-methoxy-4-hydroxybenzene

2-Methoxy-4-allylphenol

2-Methoxy-4-(2-propenyl)phenol

4-Allylguaiacol

Allylguaiacol

RN: 97-53-0 **MP (°C):** 15
MW: 164.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-02	2.463E+00	25	I019	1 0 1 2 2	
4.020E-02	6.601E+00	37	E028	1 0 1 1 2	

2143. C₁₀H₁₂O₂

Ethyl 2-phenylacetate

Phenylacetic acid ethyl ester

Ethyl benzeneacetate; ethyl phenacetate

NSC 8894

NSC 406259

Ethyl phenylacetate

RN: 101-97-3 **MP (°C):**
MW: 164.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-03	1.478E+00	25	D407	1 0 2 2 2	
8.995E-03	1.477E+00	ns	S460	0 0 0 0 0	

2144. C₁₀H₁₂O₂

β-Phenylbutyric acid

3-Phenyl-*n*-butyric acid

RN: 4593-90-2 **MP (°C):** 38
MW: 164.21 **BP (°C):** 171

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.635E-02	9.254E+00	30	D033	2 2 1 2 2	
7.013E-02	1.152E+01	40	D033	2 2 1 2 2	

2145. C₁₀H₁₂O₂*b*-Phenylethanol acetate

Phenylethyl ethanoate

b-Phenylethyl acetate

2-Phenethyl acetate; 2-phenylethyl acetate

Benzylcarbinyl acetate

NSC 71927

RN: 103-45-7 **MP (°C):**
MW: 164.21 **BP (°C):** 232

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.135E+00	25	D407	1 0 2 2 2	
1.300E-02	2.135E+00	ns	S460	0 0 0 0 0	

2146. C₁₀H₁₂O₂

2,4,6-Trimethylbenzoic acid

Mesitylenecarboxylic acid

RN: 480-63-7 **MP (°C):** 154
MW: 164.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E-03	7.225E-01	ns	C014	0 2 0 1 1	

2147. C₁₀H₁₂O₂*n*-Propyl benzoate

Propyl benzoate

Benzoicacidpropyl ester

RN: 2315-68-6 **MP (°C):** -51
MW: 164.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.531E-03	2.514E-01	20	H301	0 0 0 0 0	

2148. C₁₀H₁₂O₃

Anisyl acetate

4-Methoxybenzyl acetate

Benzinemethanol, 4-methoxy-, acetate

RN: 104-21-2 **MP (°C):**
MW: 180.21 **BP (°C):** 235

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-02	1.982E+00	25	D407	1 0 2 2 2	

2149. C₁₀H₁₂O₃

Propylparaben

Pr-paraben

Propyl *p*-hydroxybenzoic acid

Propyl 4-hydroxybenzoate

Propyl paraben

RN: 94-13-3**MP (°C):** 96.5**MW:** 180.21**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.050E-03	3.694E-01	15	B355	0 0 0 0 0	
1.172E-03	2.112E-01	15	M352	1 1 1 1 2	
2.410E-03	4.343E-01	20	B355	0 0 0 0 0	
2.055E-03	3.703E-01	25	A059	1 0 1 1 1	
2.570E-03	4.631E-01	25	B355	0 0 0 0 0	
2.773E-03	4.998E-01	25	D081	1 2 2 1 2	
1.990E-03	3.586E-01	25	D339	0 0 0 0 0	
1.778E-03	3.205E-01	25	F322	2 0 1 1 0	EFG
1.844E-03	3.323E-01	25	M352	1 1 1 1 2	
2.775E-03	5.000E-01	25	O027	1 0 1 0 0	
2.863E-03	5.160E-01	25	P013	0 0 0 0 0	
2.300E-03	4.145E-01	27	B129	2 2 2 2 1	
2.443E-03	4.403E-01	30	A059	1 0 1 1 1	
2.053E-03	3.700E-01	30	M325	1 0 0 0 1	
3.054E-03	5.503E-01	35	A059	1 0 1 1 1	
3.403E-03	6.132E-01	39.3	G302	2 2 2 2 0	EFG
4.053E-03	7.303E-01	40	A059	1 0 1 1 1	
3.925E-03	7.073E-01	40	M352	1 1 1 1 2	
6.492E-03	1.170E+00	50	M352	1 1 1 1 2	
1.515E-03	2.729E-01	ns	B404	0 2 1 1 0	

2150. C₁₀H₁₂O₄

Cantharidin

Dimethyl-3,6-epoxyperhydrophthalic anhydride

Cantharides

Hexahydro-3 α ,7 α -dimethyl-4 β ,7 β -epoxyisobenzofuran-1,3-dione

Spanish fly

RN: 56-25-7**MP (°C):****MW:** 196.20**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.529E-04	3.000E-02	20	F300	1 0 0 0 0	
3.058E-01	6.000E+01	100	F300	1 0 0 0 0	
1.514E-04	2.970E-02	ns	R427	0 0 0 0 0	

2151. C₁₀H₁₂O₅

Propyl gallate

3,4,5-Trihydroxybenzoic acid propyl ester

Gallic acid propyl ester

Progallin P

n-propyl 3,4,5-trihydroxybenzoate

Nipa 49

RN: 121-79-9**MP (°C):** 150 C**MW:** 212.20**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-02	2.792E+00	19.99	L430	0 0 0 0 0	
1.644E-02	3.488E+00	24.99	L430	0 0 0 0 0	
1.784E-02	3.786E+00	29.99	L430	0 0 0 0 0	
3.276E-02	6.951E+00	34.99	L430	0 0 0 0 0	
4.850E-02	1.029E+01	39.99	L430	0 0 0 0 0	
7.010E-02	1.488E+01	44.99	L430	0 0 0 0 0	
2.321E-01	4.925E+01	49.99	L430	0 0 0 0 0	
1.158E-01	2.458E+01	49.99	L430	0 0 0 0 0	
6.751E-01	1.432E+02	59.99	L430	0 0 0 0 0	
1.111E+00	2.357E+02	64.99	L430	0 0 0 0 0	
5.648E-03	1.199E+00	-0.	L430	0 0 0 0 0	

2152. C₁₀H₁₂O₈

Dilactone

α-Oxo-β-methylol-γ-butyrolactone betrachten

RN: MP (°C): 140**MW:** 260.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.374E-02	2.439E+01	0	F023	1 1 0 0 1	unit assumed
1.900E-01	4.943E+01	25	F023	1 1 0 0 1	unit assumed
5.972E-01	1.554E+02	50	F023	1 1 0 0 2	unit assumed
1.788E+00	4.652E+02	75	F023	1 1 0 0 2	unit assumed
2.451E+00	6.377E+02	100	F023	1 1 0 0 2	unit assumed

2153. C₁₀H₁₃ClN₂

Chlordimeform

N'-(4-Chloro-2-methylphenyl)-N,N-dimethylmethanimidamide

Bermat

Fundex

Galecon

Chlorophenamidine

RN: 6164-98-3 MP (°C): 32

MW: 196.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-03	2.030E-01	10	B324	0 0 0 0 0	
1.032E-03	2.030E-01	10	B324	0 0 0 0 0	
1.373E-03	2.700E-01	20	B300	2 0 1 1 2	
1.373E-03	2.700E-01	20	B324	0 0 0 0 0	
1.372E-03	2.699E-01	20	B324	0 0 0 0 0	
1.271E-03	2.500E-01	20	M161	1 0 0 0 2	

2154. C₁₀H₁₃ClN₂O

Trimeturon

N'-4-Chlorophenyl-O,N,N-trimethylisourea

RN: 3050-27-9 MP (°C): 147.5

MW: 212.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.289E-03	6.995E-01	ns	M061	0 0 0 0 1	

2155. C₁₀H₁₃ClN₂O

Chlortoluron

N'-(3-Chloro-4-methylphenyl)-N,N-dimethylurea

Dicuran

Chlortokem

Tolurex

RN: 15545-48-9 MP (°C): 147.5

MW: 212.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.311E-04	7.043E-02	20	B179	0 0 0 0 0	
3.291E-04	7.000E-02	20	F311	1 2 2 2 1	
3.291E-04	7.000E-02	20	M161	1 0 0 0 1	

2156. C₁₀H₁₃ClN₂O₂

Metoxuron

N'-(3-Chloro-4-methoxyphenyl)-*N,N*-dimethylurea

Purivel

Sulerex

Dosanex

Dosaflo

RN: 19937-59-8 **MP (°C):** 125**MW:** 228.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-03	6.906E-01	20	B179	0 0 0 0 0	
2.622E-03	5.996E-01	20	E048	1 2 1 1 2	
2.965E-03	6.780E-01	23	M161	0 0 0 0 2	
3.059E-03	6.995E-01	ns	B100	0 0 0 0 0	

2157. C₁₀H₁₃ClN₂O₃S

Chlorpropamide

*N*3-Butyl-*N*1-*p*-chlorobenzenesulfonylurea

Diabinese

Glucamide

Catanil

Diabaril

RN: 94-20-2 **MP (°C):** 128**MW:** 276.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.221E-03	8.913E-01	25	F415	0 0 0 0 0	
9.311E-04	2.577E-01	37	A028	1 0 2 1 2	intrinsic
9.250E-04	2.560E-01	37	A046	2 0 1 1 2	
~1.26E-03	~3.50E-01	37	B140	2 2 1 2 0	pH 1.5, form V
1.203E-03	3.330E-01	37	B140	2 2 1 2 2	pH 1.5, form I
1.384E-03	3.830E-01	37	B140	2 2 1 2 2	pH 1.5, form II
8.925E-04	2.470E-01	37	B140	2 2 1 2 2	pH 1.5, form III
1.153E-03	3.190E-01	37	B140	2 2 1 2 2	pH 1.5, form IV
>1.81E-03	>5.00E-01	ns	B404	0 2 1 1 0	
5.192E-04	1.437E-01	rt	I404	0 0 0 0 0	Average

2158. C₁₀H₁₃Cl₂FN₂O₂S₂

Tolylfluanid

1,1-Dichloro-N-((dimethylamino)sulfonyl)-1-fluoro-N-(4-methylphenyl)methanesulfenamide

Dichlofluanid-methyl

Euparen M

Bay 5712α

Bay 49854

RN: 731-27-1 **MP (°C):** 96**MW:** 347.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.570E-06	8.926E-04	ns	R427	0 0 0 0 0	
1.152E-02	4.000E+00	rt	M161	0 0 0 0 0	

2159. C₁₀H₁₃Cl₂O₃PS

Dichlofenthion

Diethyl *O*-dichlorophenyl phosphorothioate

Hexanema

Diclophenthion

Nemacide

TRI-VC13

RN: 97-17-6 **MP (°C):****MW:** 315.16 **BP (°C):** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.774E-07	2.450E-04	25	M161	1 0 0 0 2	
7.774E-07	2.450E-04	ns	F071	0 1 2 1 2	
7.774E-04	2.450E-01	ns	M061	0 0 0 0 2	sic

2160. C₁₀H₁₃FN₂O₃

1-Pivaloyloxymethyl-5-fluorouracil

RN: **MP (°C):****MW:** 228.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	2.500E+00	22	M317	1 1 1 1 1	

2161. C₁₀H₁₃FN₂O₄

1-Pivaloyloxymethyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

1-Pivaloyloxymethyl-5-fluorouracil

RN: 62113-42-2 **MP (°C):** 158-160**MW:** 244.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.418E-03	2.300E+00	22	B321	0 0 0 0 0	pH 4.0

2162. C₁₀H₁₃NO₂

Phenacetin

p-Ethoxyacetanilide*p*-Acetophenetidide**RN:** 62-44-2**MP (°C):** 134.5**MW:** 179.22**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.010E-04	5.395E-02	14	O019	1 0 0 1 2	
2.010E-03	3.603E-01	15	M352	1 1 1 1 2	
3.903E-03	6.995E-01	20	M043	1 0 0 0 0	
5.167E-03	9.261E-01	25	B434	0 0 0 0 0	
5.180E-03	9.284E-01	25	B434	0 0 0 0 0	
4.300E-02	7.706E+00	25	D044	0 0 0 0 0	
4.464E-03	8.000E-01	25	F300	1 0 0 0 0	
2.801E-03	5.020E-01	25	M333	1 1 0 0 2	
2.799E-03	5.016E-01	25	M352	1 1 1 1 2	
6.271E-03	1.124E+00	30	B434	0 0 0 0 0	
6.280E-03	1.126E+00	30	B434	0 0 0 0 0	
8.653E-03	1.551E+00	35	B434	0 0 0 0 0	
8.680E-03	1.556E+00	35	B434	0 0 0 0 0	
1.183E-02	2.120E+00	40	B434	0 0 0 0 0	
1.185E-02	2.124E+00	40	B434	0 0 0 0 0	
5.483E-03	9.828E-01	40	M352	1 1 1 1 2	
7.878E-03	1.412E+00	50	M352	1 1 1 1 2	
6.616E-02	1.186E+01	100	I315	0 0 0 0 0	
7.867E-02	1.410E+01	100	M043	1 0 0 0 2	
4.237E-03	7.594E-01	c	I315	0 0 0 0 0	
6.584E-03	1.180E+00	ns	F059	1 0 2 2 2	0.1N HCl
5.574E-03	9.990E-01	rt	D021	0 0 1 1 1	

2163. C₁₀H₁₃NO₂

Propham

Isopropyl carbanilate

Isopropyl-*N*-phenyl carbamate

IPC

RN: 122-42-9**MP (°C):** 87**MW:** 179.22**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.580E-04	1.000E-01	25	G099	1 0 0 1 0	
1.116E-04	2.000E-02	ns	B185	0 0 0 0 0	
1.786E-04	3.200E-02	ns	B185	0 0 0 0 0	
1.395E-03	2.500E-01	ns	B200	0 0 0 0 2	
5.580E-04	1.000E-01	ns	F035	0 0 0 0 0	
1.395E-03	2.500E-01	ns	H042	0 0 0 0 2	
1.000E-03	1.792E-01	ns	M163	0 0 0 0 0	EFG
1.395E-03	2.500E-01	ns	N013	0 0 0 0 2	

2164. C₁₀H₁₃NO₂

Butyl nicotinate

n-Butyl nicotinate

RN: 6938-06-3

MP (°C):

MW: 179.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.367E-02	2.450E+00	32	L346	1 0 0 1 2	

2165. C₁₀H₁₃NO₂Propyl-*p*-aminobenzoate

Risocaine

4-Aminobenzoic acid propyl ester

RN: 94-12-2

MP (°C): 75.5

MW: 179.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.655E-03	2.966E-01	15	M352	1 1 1 1 2	
2.220E-03	3.979E-01	25	H008	0 0 0 0 0	
2.860E-03	5.125E-01	25	M352	1 1 1 1 2	
3.553E-03	6.368E-01	25	P303	0 0 0 0 0	
4.219E-03	7.561E-01	33	P303	0 0 0 0 0	
4.700E-03	8.423E-01	37	F006	1 1 2 2 2	
4.629E-03	8.297E-01	40	M352	1 1 1 1 2	
5.217E-03	9.351E-01	40	P303	0 0 0 0 0	
7.047E-03	1.263E+00	50	M352	1 1 1 1 2	
1.890E-03	3.387E-01	ns	M066	0 0 0 0 2	
1.890E-03	3.387E-01	rt	B016	0 0 1 1 2	pH 7.4

2166. C₁₀H₁₃NO₂

3,4-Xylyl methylcarbamate

3,4-Dimethylphenyl methylcarbamate

3,4-Dimethylphenyl *N*-methylcarbamate

MPMC

Meobal

RN: 2425-10-7

MP (°C): 79.5

MW: 179.22

BP (°C): 126.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.254E-03	1.300E+00	30	M161	1 0 0 0 1	

2167. C₁₀H₁₃NO₂

2,6-Dimethyl-4-acetaminophenol

4-Acetamido-2,6-dimethylphenol

RN: 22900-79-4 MP (°C):

MW: 179.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-02	2.200E+00	25	D078	1 2 1 1 2	

2168. C₁₀H₁₃NO₂Methyl *p*-dimethylaminobenzoic acid

Methyl 4-dimethylaminobenzoate

RN: 1202-25-1 MP (°C): 371.7

MW: 179.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-04	6.093E-02	15	M352	1 1 1 1 2	
4.988E-04	8.940E-02	25	M352	1 1 1 1 2	
8.277E-04	1.483E-01	40	M352	1 1 1 1 2	
1.111E-03	1.991E-01	50	M352	1 1 1 1 2	

2169. C₁₀H₁₃NO₂

2,5-Dimethyl-4-acetaminophenol

4-Acetamido-2,5-dimethylphenol

RN: 69477-71-0 MP (°C):

MW: 179.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-03	1.737E+00	25	D078	1 2 1 1 2	

2170. C₁₀H₁₃NO₃*o*-Ethoxyphenyl *N*-methylcarbamate1,2-Ethoxyphenyl *N*-methylcarbamate

RN: 23409-17-8 MP (°C): 79.5

MW: 195.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.178E-02	2.300E+00	30	D089	2 2 0 0 0	

2171. C₁₀H₁₃NO₃*m*-Ethoxyphenyl *N*-methylcarbamate1,3-Ethoxyphenyl *N*-methylcarbamate**RN:** 7225-96-9 **MP (°C):** 57**MW:** 195.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.403E-03	1.250E+00	30	D089	2 2 0 0 0	

2172. C₁₀H₁₃NO₄

Methyldopa

 α -Methyldopa

Sembrina

Presinol

Sedometil

Presolisin

RN: 555-30-6 **MP (°C):** ~300**MW:** 211.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.734E-02	1.000E+01	ns	K444	0 0 0 0 0	

2173. C₁₀H₁₃N₃O₂S₂

3-Methyl-2-sulfanilamide-2,3-dihydrothiazole

Benzenesulfonamide, 4-amino-*N*-(2,3-dihydro-3-methyl-2-thiazolyl)-**RN:** 51203-20-4 **MP (°C):****MW:** 271.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.690E-04	1.544E-01	37	K095	2 0 0 0 2	intrinsic

2174. C₁₀H₁₃N₃O₅S

Nifurtimox

4-((5-Nitrofurylidene)amino)-3-methylthiomorpholine-1,1-dioxide

RN: 23256-30-6 **MP (°C):****MW:** 287.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.149E-01	3.300E+01	ns	K444	0 0 0 0 0	

2175. C₁₀H₁₃N₄O₃

Spasmolysin

 β -Hydroxypropyltheophylline

RN: 603-00-9 MP (°C):

MW: 237.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.204E+00	2.857E+02	ns	J025	0 0 0 0 1	

2176. C₁₀H₁₃N₅

4-Amino-6,7-diethylpteridine

RN: MP (°C):

MW: 203.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.171E-03	2.380E-01	20	A019	2 2 1 1 2	

2177. C₁₀H₁₃N₅

2-Amino-6,7-diethylpteridine

RN: MP (°C):

MW: 203.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.110E-04	1.852E-01	20	A019	2 2 1 1 2	

2178. C₁₀H₁₃N₅O

2-Amino-4-hydroxy-6,7-diethylpteridine

2-Amino-4-hydroxy-6:7-diethylpteridine

RN: MP (°C): >350

MW: 219.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.303E-05	1.163E-02	20	A019	2 2 1 1 2	

2179. C₁₀H₁₃N₅O

4-Amino-2-hydroxy-6,7-diethylpteridine

4-Amino-2-hydroxy-6:7-diethylpteridine

RN: MP (°C):

MW: 219.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.850E-04	6.250E-02	20	A019	2 2 1 1 2	

2180. C₁₀H₁₃N₅O₂

2',3'-Dideoxyadenosine

DDA

RN: 4097-22-7

MP (°C): 181–184

MW: 235.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.228E-01	2.890E+01	4	A337	0 0 0 0 0	
1.836E-01	4.320E+01	25	A337	0 0 0 0 0	

2181. C₁₀H₁₃N₅O₃

Deoxyadenosine

2'-Deoxyadenosine

dA

RN: 958-09-8

MP (°C):

MW: 251.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.422E-02	3.573E+00	14.88	T420	0 0 0 0 0	
1.827E-02	4.590E+00	20.26	T420	0 0 0 0 0	
2.690E-02	6.759E+00	25	H061	0 0 0 0 0	
2.558E-02	6.427E+00	25.23	T420	0 0 0 0 0	
3.683E-02	9.253E+00	29.97	T420	0 0 0 0 0	
4.780E-02	1.201E+01	35.09	T420	0 0 0 0 0	

2182. C₁₀H₁₃N₅O₄

Zidovudine

3-Azido-3-deoxythymidine

AZT

Azidodeoxythymidine

Azidothymidine

Retrovir

RN: 30516-87-1

MP (°C): 106–112

MW: 267.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.13E+00	>3.02E+02	25	B443	0 0 0 0 0	
7.521E-02	2.010E+01	ns	K444	0 0 0 0 0	
7.373E-02	1.970E+01	ns	S469	0 0 0 0 0	

2183. C₁₀H₁₃N₅O₄

Adenosine

Adenosin

9-B-D-Ribofuranosyl-9H-purin-6-amine adenine riboside

Adenocard

9-β-D-Ribofuranosyladenine

RN: 58-61-7 **MP (°C):** 234**MW:** 267.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	5.131E+00	25	H061	0 0 0 0 0	
2.000E-02	5.345E+00	ns	R030	0 0 0 0 0	
1.905E-02	5.092E+00	ns	R427	0 0 0 0 0	
8.232E-05	2.200E-02	rt	N015	0 0 2 2 1	sic

2184. C₁₀H₁₃N₅O₄

Guanine deoxyriboside

RN: 961-07-9 **MP (°C):****MW:** 267.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.680E-03	1.785E+00	14.88	T420	0 0 0 0 0	
8.790E-03	2.349E+00	20.26	T420	0 0 0 0 0	
1.118E-02	2.988E+00	25.02	T420	0 0 0 0 0	
1.589E-02	4.247E+00	29.97	T420	0 0 0 0 0	
2.072E-02	5.537E+00	35.09	T420	0 0 0 0 0	

2185. C₁₀H₁₃N₅O₅

Guanosine

Guanosin

2-Amino-9-β-D-ribofuranosyl-9H-purine-6-(1H)-one

Guanine riboside

rG

RN: 118-00-3 **MP (°C):** 250**MW:** 283.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.471E-03	7.000E-01	18	F300	1 0 0 0 1	
4.300E-03	1.218E+00	25	C416	2 1 1 1 1	
1.820E-03	5.155E-01	25	H061	0 0 0 0 0	
1.073E-01	3.040E+01	100	F300	1 0 0 0 1	

2186. C₁₀H₁₄

Isobutylbenzene

2-Methyl-1-phenylpropane

(2-Methylpropyl)-benzene

RN: 538-93-2 **MP (°C):** -51
MW: 134.22 **BP (°C):** 170.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.525E-05	1.010E-02	25	P051	2 1 1 2 2	
7.525E-05	1.010E-02	25.00	P007	2 1 2 2 2	
7.525E-05	1.010E-02	ns	H123	0 0 0 0 0	

2187. C₁₀H₁₄

Durene

1,2,4,5-Tetramethylbenzene

Durol

RN: 95-93-2 **MP (°C):** 80.0
MW: 134.22 **BP (°C):** 192.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.593E-05	3.480E-03	25	K119	1 0 0 0 2	
2.593E-05	3.480E-03	25	P051	2 1 1 2 2	
2.593E-05	3.480E-03	25.00	P007	2 1 2 2 2	
1.445E-04	1.940E-02	ns	D001	0 0 0 0 2	
7.152E-05	9.600E-03	ns	H123	0 0 0 0 0	

2188. C₁₀H₁₄

Butylbenzene

1-Phenylbutane

n-Butylbenzene

RN: 68411-44-9 **MP (°C):** -88
MW: 134.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	1.745E+00	ns	H307	0 0 0 0 0	

2189. C₁₀H₁₄*n*-Butylbenzene

1-Phenylbutane

Butylbenzene

RN: 104-51-8**MP (°C):** -88.5**MW:** 134.22**BP (°C):** 183.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.940E-05	1.334E-02	7	O312	2 2 0 2 2	
9.670E-05	1.298E-02	10	O312	2 2 0 2 2	
9.790E-05	1.314E-02	12.5	O312	2 2 0 2 2	
9.660E-05	1.297E-02	15	O312	2 2 0 2 2	
9.790E-05	1.314E-02	17.5	O312	2 2 0 2 2	
9.909E-05	1.330E-02	20	B356	0 0 0 0 0	
1.018E-04	1.366E-02	20	O312	2 2 0 2 2	
9.387E-06	1.260E-03	25	A002	1 2 1 1 2	<i>sic</i>
3.700E-04	4.966E-02	25	K001	1 0 2 1 2	
1.320E-04	1.772E-02	25	M124	2 1 2 2 2	
1.030E-04	1.382E-02	25	M342	1 0 1 1 2	
1.025E-04	1.376E-02	25	O312	2 2 0 2 2	
8.791E-05	1.180E-02	25	S005	2 2 2 2 2	
3.725E-04	5.000E-02	25	S012	2 0 2 2 0	
8.791E-05	1.180E-02	25	S191	1 2 2 2 2	
8.791E-05	1.180E-02	25	S358	2 1 2 2 2	
1.030E-04	1.382E-02	25	W300	2 2 2 2 2	
1.244E-04	1.670E-02	29.99	C350	0 0 0 0 0	
1.086E-04	1.458E-02	30	O312	2 2 0 2 2	
1.147E-04	1.540E-02	35	O312	2 2 0 2 2	
1.328E-04	1.782E-02	39.99	C350	0 0 0 0 0	
1.234E-04	1.656E-02	40	O312	2 2 0 2 2	
1.411E-04	1.894E-02	45	O312	2 2 0 2 2	
1.517E-04	2.036E-02	49.99	C350	0 0 0 0 0	
2.006E-04	2.692E-02	59.99	C350	0 0 0 0 0	
2.389E-04	3.206E-02	69.99	C350	0 0 0 0 0	
3.555E-04	4.772E-02	79.99	C350	0 0 0 0 0	
4.555E-04	6.114E-02	89.99	C350	0 0 0 0 0	
6.222E-04	8.351E-02	99.99	C350	0 0 0 0 0	
9.387E-05	1.260E-02	ns	H123	0 0 0 0 0	

2190. C₁₀H₁₄*p*-Cymene

1-Methyl-4-isopropylbenzene

4-Cymene

Dolcymine

RN: 99-87-6**MP (°C):** -68**MW:** 134.22**BP (°C):** 177

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.979E-03	3.998E-01	25	B019	1 0 1 2 0	<i>sic</i>
1.740E-04	2.335E-02	25	B173	2 0 2 2 2	<i>sic</i>

2191. C₁₀H₁₄

sec-Butylbenzene

1-Methylpropylbenzene

RN: 135-98-8 **MP (°C):** -82.7
MW: 134.22 **BP (°C):** 173.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.302E-03	3.090E-01	25	A002	1 2 1 1 2	<i>sic</i>
7.525E-05	1.010E-02	25	K119	1 0 0 0 2	
1.311E-04	1.760E-02	25	S005	2 2 2 2 2	
1.311E-04	1.760E-02	25	S191	1 2 2 2 2	
1.311E-04	1.760E-02	25	S358	2 1 2 2 2	

2192. C₁₀H₁₄

tert-Butylbenzene

1,1-Dimethylethylbenzene

t-Butylbenzene

RN: 98-06-6 **MP (°C):** -58
MW: 134.22 **BP (°C):** 168.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.533E-04	3.400E-02	25	A002	1 2 1 1 1	
2.198E-04	2.950E-02	25	S005	2 2 2 2 2	
1.311E-04	1.760E-02	25	S191	1 2 2 2 2	
2.198E-04	2.950E-02	25	S358	2 1 2 2 2	

2193. C₁₀H₁₄

1,2-Diethylbenzene

o-Diethylbenzene

RN: 135-01-3 **MP (°C):** -31
MW: 134.22 **BP (°C):** 183

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	7.114E-02	10	B149	2 1 1 2 1	
5.300E-04	7.114E-02	20	B149	2 1 1 2 1	

2194. C₁₀H₁₄

1,4-Diethylbenzene

p-Diethylbenzene

RN: 105-05-5 **MP (°C):** -43
MW: 134.22 **BP (°C):** 184

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	2.483E-02	10	B149	2 1 1 2 2	
1.850E-04	2.483E-02	20	B149	2 1 1 2 2	

2195. C₁₀H₁₄Cl₂NO₂PS

DMPA

Isopropylphosphoramidothioate

O-(2,4-Dichlorophenyl)-O-methyl

Phosphoramidothioic acid, isopropyl-*o*-(2,4-dichlorophenyl)-*o*-methyl ester

RN: 299-85-4 MP (°C): 51.4

MW: 314.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.595E-05	5.010E-03	25	B185	0 0 0 0 0	
1.591E-05	5.000E-03	25	B200	1 0 0 0 0	
1.591E-05	5.000E-03	ns	M061	0 0 0 0 0	

2196. C₁₀H₁₄Cl₆N₄O₂

Triforine

N,N'-[1,4-Piperazinediylbis(2,2,2-trichloroethylidene)] bisformamide

Funginex

Denarin

Biformylchlorazin

Saprol

RN: 26644-46-2 MP (°C): 155

MW: 434.97 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.38E-05	~6.00E-03	rt	D303	0 0 0 0 0	
6.437E-05	2.800E-02	rt	M161	0 0 0 0 0	

2197. C₁₀H₁₄NO₅PS

Parathion

O,O-Diethyl O-*p*-nitrophenyl phosphorothioate

Foliclal

Rhodiatox

Alkron

Fosferno

RN: 56-38-2 MP (°C): 6

MW: 291.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.536E-05	1.030E-02	10	B324	0 0 0 0 0	
3.536E-05	1.030E-02	10	B324	0 0 0 0 0	
4.257E-05	1.240E-02	20	B169	2 1 1 1 1	
8.318E-05	2.423E-02	20	B179	0 0 0 0 0	
4.429E-05	1.290E-02	20	B324	0 0 0 0 0	
4.429E-05	1.290E-02	20	B324	0 0 0 0 0	
2.245E-05	6.540E-03	24	F179	2 2 2 2 2	
8.240E-05	2.400E-02	25	M161	1 0 0 0 1	

(continued)

2197. C₁₀H₁₄NO₅PS (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.219E-05	1.520E-02	30	B324	0 0 0 0 0	
5.219E-05	1.520E-02	30	B324	0 0 0 0 0	
4.086E-05	1.190E-02	ns	F071	0 1 2 1 2	
8.240E-05	2.400E-02	ns	M061	0 0 0 0 1	
6.867E-05	2.000E-02	ns	M110	0 0 0 0 0	EFG
8.240E-05	2.400E-02	ns	M344	0 0 0 0 1	

2198. C₁₀H₁₄NO₆P

Paraoxon

Diethyl *p*-nitrophenyl phosphate

Fosfacol

Eticol

Ethyl paraoxon

Miotisal

RN: 311-45-5 MP (°C):

MW: 275.20 BP (°C): 169–170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.318E-02	3.627E+00	20	B169	2 0 1 1 2	
3.634E-03	1.000E+00	20	F300	1 0 0 0 0	

2199. C₁₀H₁₄N₂O

N-(Dimethylaminomethyl)benzamide

Benzamide, *N*-[(dimethylamino)methyl]-

RN: 59917-58-7 MP (°C):

MW: 178.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E+00	4.634E+02	22	J037	0 0 0 0 0	

2200. C₁₀H₁₄N₂O

N-(Ethylaminomethyl)benzamide

Benzamide, *N*-[(ethylamino)methyl]-

RN: 73239-20-0 MP (°C):

MW: 178.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-02	1.301E+01	22	J037	0 0 0 0 0	

2201. C₁₀H₁₄N₂O₂

m-N,N-Dimethylaminophenyl *N*-methylcarbamate
1,3-N,N-Dimethylaminophenyl *N*-methylcarbamate

RN: 2631-39-2 **MP (°C):** 86
MW: 194.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.604E-03	7.000E-01	30	D089	2 2 0 0 0	

2202. C₁₀H₁₄N₂O₃

5-Methyl-5-(3-methylbut-2-enyl)barbituric acid
2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-(3-methyl-2-but enyl)
5-Methyl-5-(3-methylbut-2-enyl)barbiturate

RN: 66843-01-4 **MP (°C):**
MW: 210.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.503E-03	5.262E-01	25	P350	0 0 0 0 0	intrinsic

2203. C₁₀H₁₄N₂O₃

2,4-Diazaspiro[5.6]dodecane-1,3,5-trione
Cycloheptane-spirobarbiturate

RN: 143288-61-3 **MP (°C):**
MW: 210.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.790E-04	1.427E-01	25	P350	0 0 0 0 0	intrinsic

2204. C₁₀H₁₄N₂O₃

5-Isopropyl-5-allylbarbituric acid
Aprobarbital

5-(1-Methylethyl)-5-(2-propenyl)-2,4,6(1H,3H,5H)-pyrimidinetrione
5-Allyl-5-isopropylbarbituric acid

Aprobarbitone
RN: 77-02-1 **MP (°C):** 141
MW: 210.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.617E-02	3.400E+00	20	J030	1 2 2 2 2	
1.960E-02	4.121E+00	25	P350	0 0 0 0 0	intrinsic
1.940E-02	4.079E+00	25	V033	2 0 1 1 2	
1.940E-02	4.079E+00	25.00	T303	1 0 0 0 2	
2.600E-02	5.466E+00	35.00	T303	1 0 0 0 2	
2.664E-02	5.600E+00	37	J030	1 2 2 2 2	
3.340E-02	7.022E+00	45.00	T303	1 0 0 0 2	
1.912E-02	4.020E+00	ns	T003	0 0 0 0 2	

2205. C₁₀H₁₄N₂O₅

Thymidine

(1-[2-Deoxy-β-D-ribofuranosyl]-5-methyluracil)

Thyminedeoxyriboside

2'-deoxy-5-methyl

Thymine-2-desoxyriboside

Uridine

RN: 50-89-5

MP (°C): 187–189

MW: 242.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.720E-02	6.589E+00	19.99	T418	0 0 0 0 0	
2.790E-02	6.758E+00	24.96	T418	0 0 0 0 0	
2.780E-02	6.734E+00	24.99	T418	0 0 0 0 0	
3.040E-02	7.364E+00	24.99	T418	0 0 0 0 0	
2.790E-02	6.758E+00	24.99	T418	0 0 0 0 0	
2.870E-02	6.952E+00	24.99	T418	0 0 0 0 0	
2.200E-01	5.329E+01	24.99	T418	0 0 0 0 0	
2.710E-02	6.565E+00	25.49	T418	0 0 0 0 0	

2206. C₁₀H₁₄N₂S

Methiuron

N,N-Dimethyl-N'-3-methylphenylthiourea

RN: 21540-35-2 MP (°C): 145

MW: 194.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.059E-03	4.000E-01	ns	M061	0 0 0 0 2	

2207. C₁₀H₁₄N₄O₂

7-Propyl theophylline

3,7-Dimethyl-7-propyl-xanthine

RN: 27760-74-3 MP (°C):

MW: 222.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E+00	2.320E+02	30	B042	1 2 1 1 2	
1.040E+00	2.311E+02	30	G021	1 0 0 0 2	

2208. C₁₀H₁₄N₄O₂

1-Propyl theobromine

3,7-Dimethyl-1-propyl-xanthine

RN: 204443-29-8 MP (°C): 99

MW: 222.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.190E-02	1.376E+01	30	B042	1 2 1 1 2	

2209. C₁₀H₁₄N₄O₃

Ethoxycaffeine

1,3,7-Trimethyl-2,6-dioxo-8-ethoxypurine

RN: 577-66-2 MP (°C): 143

MW: 238.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.255E-02	2.991E+00	19	A072	1 2 1 0 1	

2210. C₁₀H₁₄N₄O₄

Diphylline

7-(2,3-Dihydroxypropyl)theophylline

Lufyllin-EPG

Neothylline

Airet

RN: 479-18-5 MP (°C): 158

MW: 254.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.686E-01	1.700E+02	37	F076	2 0 2 2 1	

2211. C₁₀H₁₄N₅O₇P

2'-Adenylic acid

2'-Adenylsaeure

RN: 130-49-4 MP (°C):

MW: 347.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-03	5.000E-01	15	F300	1 0 0 0 0	

2212. C₁₀H₁₄N₅O₇P

3'-Adenylic acid

3'-Adenylsaeure

RN: 84-21-9 MP (°C): 197

MW: 347.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-03	5.000E-01	15	F300	1 0 0 0 0	

2213. C₁₀H₁₄O

L-Carvone

r-(*-*)-Mentha-6,8-dien-2-one

1-Methyl-4-isopropenyl-6-cyclohexen-2-one

p-Mentha-6,8-dien-2-one

RN: 6485-40-1 MP (°C): <25

MW: 150.22 BP (°C): 230

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.654E-03	1.300E+00	18	F300	1 0 0 0 1	
8.654E-03	1.300E+00	25	A049	1 0 0 0 1	
1.020E-02	1.532E+00	25	A401	1 0 2 2 0	
1.100E-02	1.652E+00	25	D407	1 0 2 2 2	
1.100E-02	1.652E+00	37	E028	1 0 1 1 2	

2214. C₁₀H₁₄O

l-Perillaldehyde

4-Isopropenyl-1-cyclohexene-1-carboxaldehyde

para-Mentha-1,8-dien-7-al

L-4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde

L(-)-Perillaldehyde

(S)-4-(1-Methylethenyl)-1-cyclohexene-1-carboxaldehyde

RN: 18031-40-8 MP (°C):

MW: 150.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	6.309E-01	25	A401	1 0 2 2 0	

2215. C₁₀H₁₄O*p*-n-Butylphenol

4-n-Butylphenol

RN: 1638-22-8 MP (°C):

MW: 150.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.038E-03	4.563E-01	20	R087	0 0 0 0 0	0.15M NaCl
2.662E-03	3.998E-01	25	L022	1 0 0 0 0	

2216. C₁₀H₁₄O*o*-n-Butylphenol

2-n-Butylphenol

RN: 28805-86-9 MP (°C):

MW: 150.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.662E-03	3.998E-01	25	L022	1 0 0 0 0	

2217. C₁₀H₁₄O*p-tert-Butylphenol**4-t-Butylphenol*

RN: 98-54-4

MP (°C): 99.5

MW: 150.22

BP (°C): 237

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.327E-03	6.500E-01	22.5	G301	0 0 0 0 0	
3.327E-03	4.998E-01	25	L021	1 0 0 0 0	
3.861E-03	5.800E-01	25	M127	1 0 0 0 1	
4.427E-03	6.650E-01	25	P004	0 0 0 0 0	
5.076E-03	7.625E-01	30	P004	0 0 0 0 0	
5.785E-03	8.690E-01	35	P004	0 0 0 0 0	
6.534E-03	9.815E-01	40	P004	0 0 0 0 0	
4.266E-03	6.408E-01	ns	R427	0 0 0 0 0	

2218. C₁₀H₁₄O*Thymol**6-Isopropyl-*m*-cresol**3-Hydroxy-*p*-cymene**5-Methyl-2-isopropyl-1-phenol**2-Isopropyl-5-methyl phenol**5-Methyl-2-(1-methylethyl)phenol*

RN: 89-83-8 MP (°C): 48–51

MW: 150.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.991E-03	9.000E-01	20	F300	1 0 0 0 0	
6.000E-03	9.013E-01	25	D407	1 0 2 2 2	
5.700E-03	8.563E-01	25	F044	1 0 0 0 1	
6.046E-03	9.083E-01	25	L021	1 0 0 0 0	
6.650E-03	9.990E-01	25	R041	0 0 0 0 0	
5.990E-02	8.998E+00	37	E028	1 0 1 1 2	<i>sic</i>
8.654E-03	1.300E+00	37	F300	1 0 0 0 1	
6.166E-03	9.263E-01	ns	R427	0 0 0 0 0	

2219. C₁₀H₁₄O*Carvacrol**2-Methyl-5-isopropylphenol*

RN: 499-75-2 MP (°C): 3

MW: 150.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.650E-03	9.990E-01	25	L021	1 0 0 0 0	
8.321E-03	1.250E+00	25	M127	1 0 0 0 2	

2220. C₁₀H₁₄O4-*sec*-Butylphenol*p*-*sec*-Butylphenol

RN: 99-71-8

MP (°C):

MW: 150.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.391E-03	9.600E-01	25	M127	1 0 0 0 1	

2221. C₁₀H₁₄O₂

3-Butoxyphenol

m-Butoxy phenol

Phenol, 3-butoxy-

RN: 18979-72-1 MP (°C):

MW: 166.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.240E-03	1.370E+00	30	B315	0 0 0 0 0	

2222. C₁₀H₁₄O₂*p*-Diethoxybenzene

4-Diethoxybenzene

RN: 122-95-2 MP (°C):

MW: 166.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.560E-04	7.580E-02	25	C316	0 0 0 0 0	0.1M NaCl

2223. C₁₀H₁₄O₂*o*-Butoxyphenol

2-Butoxyphenol

RN: 39075-90-6 MP (°C):

MW: 166.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.920E-03	6.516E-01	24.99	B353	0 0 0 0 0	

2224. C₁₀H₁₄O₈

1,1,2,2-Ethanetetrol, tetraacetate

Glyoxal-tetraacetat

Glyoxal tetraacetate

RN: 59602-16-3 **MP (°C):****MW:** 262.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.051E-05	8.000E-03	25	F300	1 0 0 0 1	

2225. C₁₀H₁₅N

Diethylaniline

2,6-Diethylaniline

RN: 579-66-8 **MP (°C):** -38**MW:** 149.24 **BP (°C):** 215

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.489E-03	6.700E-01	26.70	L095	2 2 1 1 2	
4.467E-03	6.666E-01	ns	S460	0 0 0 0 0	

2226. C₁₀H₁₅NO

Ethyl phenyl ethanolamine

2-(*N*-Ethylanilino)ethanol*N*-Phenyl-*N*-ethyl ethanolamine**RN:** 92-50-2 **MP (°C):****MW:** 165.24 **BP (°C):** 268

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.011E-02	4.975E+00	20	M062	1 0 0 0 1	

2227. C₁₀H₁₅NO

Ephedrine

L-Erythro-2-(methylamino)-1-phenylpropan-1-ol

(1*R*,2*S*)-(−)-Ephedrine

L-α-(1-Methylaminoethyl)benzyl alcohol

RN: 299-42-3 **MP (°C):** 38–39**MW:** 165.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.882E-01	4.762E+01	25	D004	0 0 0 0 0	
3.442E-01	5.688E+01	25	L338	1 0 1 1 2	
3.850E-01	6.362E+01	30	L069	1 0 1 1 0	EFG
1.160E+00	1.917E+02	ns	F007	0 0 0 0 2	

2228. C₁₀H₁₅NO

(+) -Pseudoephedrine

(+) -Pseudoephedrin

RN: 90-82-4**MP (°C):** 118**MW:** 165.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.03E-03	<5.00E-01	rt	B435	0 0 0 0 0	

2229. C₁₀H₁₅NO₂

N-Phenyl diethanolamine

Phenyl diethanolamine

N,N-di(Hydroxyethyl)aniline

2,2'-(Phenylimino)diethanol

PDEA

RN: 120-07-0**MP (°C):** 57**MW:** 181.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-01	3.232E+01	20	M062	1 0 0 0 2	

2230. C₁₀H₁₅N₅O₅

Arabinosyladenine

9-β-D-Arabinofuranosyl adenine

Vidarabine

β-D-Arabinosyladenine

Spongoadenosine

RN: 24356-66-9**MP (°C):** 208**MW:** 285.26**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	5.135E-01	ns	R030	0 0 0 0 0	

2231. C₁₀H₁₅OPS₂

Fonofos

Ethyl S-phenyl ethylphosphonothiolthionate

Diphonate

Dyfonate®

Stauffer N-2790

RN: 944-22-9**MP (°C):****MW:** 246.33**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.373E-05	1.570E-02	20	B169	2 1 1 1 2	
6.089E-05	1.500E-02	ns	M110	0 0 0 0 0	EFG

(continued)

2231. C₁₀H₁₅OPS₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.272E-05	1.299E-02	ns	S460	0 0 0 0 0	
6.374E-05	1.570E-02	ns	V414	0 0 0 0 0	

2232. C₁₀H₁₅O₃PS₂

Fenthion

4-Methylmercapto-3-methylphenyl dimethyl thiophosphate

Mercaptosfos

Thiophos

Baycid

Entex

RN: 55-38-9 MP (°C): 7.5

MW: 278.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.299E-05	6.400E-03	10	B324	0 0 0 0 0	
2.300E-05	6.402E-03	10	B324	0 0 0 0 0	
2.698E-05	7.509E-03	20	B300	2 1 1 1 2	
3.244E-05	9.029E-03	20	B324	0 0 0 0 0	
3.341E-05	9.300E-03	20	B324	0 0 0 0 0	
1.940E-04	5.400E-02	20	M061	1 0 0 0 1	
4.074E-05	1.134E-02	30	B324	0 0 0 0 0	
4.060E-05	1.130E-02	30	B324	0 0 0 0 0	
1.976E-04	5.500E-02	rt	M161	0 0 0 0 0	

2233. C₁₀H₁₆

Myrcene

7-Methyl-3-methylene-1,6-octadiene

7-Methyl-3-methylene-1,6-octadiene

7-Methyl-3-methyleneocta-1,6-diene

7-Methyl-3-methylene-octadiene

β-Myrcene

RN: 123-35-3 MP (°C):

MW: 136.24 BP (°C): 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	4.087E-03	25	A401	1 0 2 2 0	
7.560E-05	1.030E-02	25	L450	0 0 0 0 0	

2234. C₁₀H₁₆ β -Pinene

(10)-Pinene

Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-

Nopinene

Pseudopinene

RN: 127-91-3 **MP (°C):** -61**MW:** 136.24 **BP (°C):** 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.333E-05	1.272E-02	24.99	T424	0 0 0 0 0	
8.808E-05	1.200E-02	25	L450	0 0 0 0 0	

2235. C₁₀H₁₆

D-Limonene

D-1,8-*p*-Menthadiene

(R)-1-Methyl-4-(1-methylethenyl)cyclohexene

(R)-(+)-Limonene

Hemo-sol

RN: 5989-27-5 **MP (°C):** 95**MW:** 136.24 **BP (°C):** 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.080E-01	9.646E+01	0	M124	2 1 2 2 1	
7.670E-01	1.045E+02	5	M124	2 1 2 2 2	
6.973E-05	9.500E-03	25	L450	0 0 0 0 0	
1.011E-04	1.377E-02	25	M124	2 1 2 2 1	

2236. C₁₀H₁₆

Limonene

p-Mentha-1,8-diene

Cyclil decene

Acintene DP dipentene

RN: 138-86-3 **MP (°C):** 73.97**MW:** 136.24 **BP (°C):** 175.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-05	4.332E-03	6	P430	0 0 0 0 0	
4.100E-05	5.586E-03	23.5	P430	0 0 0 0 0	
9.055E-05	1.234E-02	24.99	T424	0 0 0 0 0	
6.390E-05	8.706E-03	25	I019	1 0 1 2 2	
2.202E-04	3.000E-02	25	M350	1 0 1 1 1	

2237. C₁₀H₁₆ γ -Terpinene

1-Methyl-4-(1-methylethyl)-1,4-cyclohexadiene

1,4-*p*-Menthadiene

1-Isopropyl-4-methyl-1,4-cyclohexadiene

Moslene

Terpinene

RN: 99-85-4**MP (°C):****MW:** 136.24**BP (°C):** 182

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-05	6.090E-03	6	P430	0 0 0 0 0	
6.370E-05	8.678E-03	23.5	P430	0 0 0 0 0	

2238. C₁₀H₁₆

Terpinolene

1-Methyl-4-(1-methylethylidene)cyclohexene

1,4(8)-*p*-Menthadiene

1-Methyl-4-(1-methylethylidene)cyclohexene

Terpinolene 30/35

Terpinolene 90

RN: 586-62-9**MP (°C):****MW:** 136.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.670E-05	7.725E-03	6	P430	0 0 0 0 0	
6.960E-05	9.482E-03	23.5	P430	0 0 0 0 0	
5.000E-05	6.812E-03	25	A401	1 0 2 2 0	

2239. C₁₀H₁₆ α -Pinene

2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene

Acitene A

Cyclic dextadiene

pin-2(3)-ene

2-Pinene

RN: 80-56-8**MP (°C):** -64**MW:** 136.24**BP (°C):** 155

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.670E-05	2.275E-03	6	P430	0 0 0 0 0	
1.830E-05	2.493E-03	23.5	P430	0 0 0 0 0	
3.867E-05	5.268E-03	24.99	T424	0 0 0 0 0	
3.523E-05	4.800E-03	25	L450	0 0 0 0 0	

2240. C₁₀H₁₆Cl₃NOS

Triallate

S-(2,3,3-Trichloroallyl)diisopropylthiocarbamate

RN: 2303-17-5 MP (°C): 29

MW: 304.67 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.313E-05	4.000E-03	25	B200	1 0 0 1 0	
1.313E-05	4.000E-03	25	M161	1 0 0 0 0	
1.313E-05	4.000E-03	ns	F019	0 0 0 0 0	

2241. C₁₀H₁₆NO₂S₂

2-Cyclopentamethylene-4-methoxycarbamyl-1,3-dithiolane

2-Cyclopentyl-4-methoxycarbamyl-1,3-dithiolane

RN: MP (°C):

MW: 246.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	7.391E-02	rt	B174	0 0 1 0 0	

2242. C₁₀H₁₆NO₃S

2-Cyclopentamethylene-4-methoxycarbamyl-1,3-oxathiolane

RN: MP (°C):

MW: 230.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-03	3.455E-01	rt	B174	0 0 1 0 1	

2243. C₁₀H₁₆NO₄

2-Cyclopentamethylene-4-methoxycarbamyl-1,3-dioxolane

RN: MP (°C):

MW: 214.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	2.785E+00	rt	B174	0 0 1 0 1	

2244. C₁₀H₁₆N₂O₃

5-Ethyl-5-(2-methylpropyl)barbituric acid

RN: 125-40-6 MP (°C): 174.5

MW: 212.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.997E-03	8.483E-01	25	B065	1 2 1 1 1	

2245. C₁₀H₁₆N₂O₃

5,5-Dipropylbarbituric acid

5,5-Dipropylbarbitursaeure

Proponal

5,5-Dipropylbarbiturate

RN: 2217-08-5 MP (°C): 146

MW: 212.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-03	6.000E-01	20	F300	1 0 0 0 0	
2.968E-03	6.300E-01	20	J030	1 2 2 2 1	
5.088E-03	1.080E+00	37	J030	1 2 2 2 2	
6.926E-02	1.470E+01	100	F300	1 0 0 0 2	

2246. C₁₀H₁₆N₂O₃

5,5-Diisopropylbarbituric acid

Barbituric acid, 5,5-diisopropyl

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-bis(1-methylethyl)

5,5-Di-i-propylbarbiturate

RN: 99167-69-8 MP (°C):

MW: 212.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.715E-03	3.640E-01	25	P350	0 0 0 0 0	intrinsic

2247. C₁₀H₁₆N₂O₃

Butabarbital

Butethal

5-Ethyl-5-n-butylbarbituric acid

5-Butyl-5-ethylbarbituric acid

RN: 77-28-1 MP (°C): 127

MW: 212.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.602E-02	3.400E+00	0	D089	0 0 0 0 2	form I
1.484E-02	3.150E+00	20	J030	1 2 2 2 2	
1.044E-02	2.215E+00	20	K078	1 0 2 1 2	
4.052E-03	8.600E-01	25	B011	2 0 0 1 0	
4.218E-03	8.954E-01	25	B065	1 1 1 1 1	
1.936E-02	4.110E+00	25	B065	1 1 1 1 1	
8.000E-03	1.698E+00	25	G003	1 1 1 1 1	pH 4.7
2.300E-02	4.882E+00	25	M310	2 2 2 2 2	
2.130E-02	4.521E+00	25	V033	2 0 1 1 2	
4.070E-03	8.639E-01	25	V033	2 0 1 1 2	
2.130E-02	4.521E+00	25.00	T303	1 0 0 0 2	
7.400E-03	1.571E+00	25.00	T303	1 0 0 0 1	

(continued)

2247. C₁₀H₁₆N₂O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-02	4.139E+00	30	I001	2 0 2 1 0	EFG, 0.003N H ₂ SO ₄
9.900E-03	2.101E+00	35.00	T303	1 0 0 0 1	
2.430E-02	5.158E+00	35.00	T303	1 0 0 0 2	
2.299E-02	4.880E+00	37	J030	1 2 2 2 2	
3.090E-02	6.559E+00	45.00	T303	1 0 0 0 2	
1.370E-02	2.908E+00	45.00	T303	1 0 0 0 2	
1.743E-02	3.700E+00	amb	D092	0 2 2 1 2	form II
1.602E-02	3.400E+00	amb	D092	0 2 2 1 2	0.1N HCl, form III, mp 124 C
1.743E-02	3.700E+00	amb	D092	0 2 2 1 2	form I
9.362E-03	1.987E+00	ns	T003	0 0 0 0 2	
8.952E-03	1.900E+00	ns	T003	0 0 0 0 2	

2248. C₁₀H₁₆N₂O₃S

Biotin d

D-Biotin

Biotin

RN: 58-85-5 **MP (°C):** 232
MW: 244.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.003E-04	2.200E-01	25	D041	1 0 0 0 1	
1.433E-03	3.500E-01	25	D315	0 0 0 0 0	
8.186E-04	2.000E-01	25	M054	1 0 0 0 0	

2249. C₁₀H₁₆N₂O₄

Methyl-2,2-diallylmalonurate

Methyl 2,2-diallylmalonurate

RN: 73632-82-3 **MP (°C):** 84
MW: 228.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	1.552E+00	23	B152	1 2 1 1 1	pH 3.5

2250. C₁₀H₁₆N₄O₂

7-Butyl theophylline

1H-Purine-2,6-dione, 7-butyl-3,7-dihydro-1,3-dimethyl-

7-Butyl-1,3-dimethylxanthine

RN: 1021-65-4 **MP (°C):**
MW: 224.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.560E-02	3.499E+00	30	B042	1 2 1 1 2	
1.560E-02	3.499E+00	30	G021	1 0 0 0 2	

2251. C₁₀H₁₆N₄O₂S3-(5-*tert*-Butyl-1,3,4-thiadiazol-2-yl)-4-hydroxy-1

2-Imidazolidinone, 3-[5-(1,1-dimethylethyl)-1,3,4-thiadiazol-2-yl]-4-hydroxy-1-methyl-Buthidazole

Ravage

VEL 5026

RN: 55511-98-3 **MP (°C):** 133.5
MW: 256.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.322E-02	3.388E+00	25	M161	1 0 0 0 1	

2252. C₁₀H₁₆N₆S

Cimetidine

2-Cyano-1-methyl-3-(2-(((5-methylimidazol-4-yl)methyl)thio)ethyl)guanidine

N"-Cyano-N-methyl-N'-(2-(((5-methyl-1H-imidazol-4-yl)methyl)thio)-ethyl)guanidine

N"-Cyano-N-methyl-N'-(2-(((5-methyl-1H-imidazol-4-yl)methyl)thio)-ethyl)guanidine

Sigmetadine

Peptol

RN: 51481-61-9 **MP (°C):** 142
MW: 252.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.382E-02	6.010E+00	22.5	B422	2 0 2 2 2	
3.685E-02	9.300E+00	25	A412	1 0 2 2 1	int
3.963E-03	1.000E+00	ns	K444	0 0 0 0 0	

2253. C₁₀H₁₆O

D-Fenchone

D-1,3,3-Trimethyl-2-norbornanone

Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimethyl-, (1S)-

α-Fenchone

(+)Fenchone

RN: 4695-62-9 **MP (°C):** 6.1
MW: 152.24 **BP (°C):** 193.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-02	1.996E+00	20	D052	1 1 0 0 0	
1.410E-02	2.147E+00	25	I019	1 0 1 2 2	
1.413E-02	2.150E+00	ns	S460	0 0 0 0 0	

2254. C₁₀H₁₆O

D-Camphor

D-Campher

Camphor

RN: 76-22-2**MP (°C):** 179.7**MW:** 152.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	1.667E+00	15.50	L073	1 2 2 1 2	
6.569E-03	1.000E+00	20	F300	1 0 0 0 0	
1.363E-02	2.076E+00	20	K078	1 0 2 1 2	
1.030E-02	1.568E+00	25	I019	1 0 1 2 2	
1.340E-02	2.040E+00	25	L338	1 0 1 1 2	
1.630E-02	2.481E+00	37	E028	1 0 1 1 2	
1.115E-02	1.697E+00	ns	F014	0 0 0 0 2	
1.023E-02	1.558E+00	ns	R427	0 0 0 0 0	

2255. C₁₀H₁₆O

Carvotan acetone

Carvotan-aceton

RN: 499-71-8**MP (°C):****MW:** 152.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.912E-03	9.000E-01	20	F300	1 0 0 0 0	

2256. C₁₀H₁₆O

Citral

trans-3,7-dimethyl-2,6-octadienal

Geranaldehyde

Neral

Geranial

Citral A

RN: 5392-40-5**MP (°C):** <10**MW:** 152.24**BP (°C):** 92.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-03	5.785E-01	25	A401	1 0 2 2 0	
1.583E-03	2.410E-01	25	L450	0 0 0 0 0	
1.970E-03	2.999E-01	25	M350	1 0 1 1 1	
8.800E-03	1.340E+00	37	E028	1 0 1 1 1	
8.710E-03	1.326E+00	ns	S460	0 0 0 0 0	

2257. C₁₀H₁₆O

L-Dihydrocarvone

L-Dihydro-carvon

RN: 619-02-3

MP (°C):

MW: 152.24

BP (°C): 221

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.569E-03	1.000E+00	20	F300	1 0 0 0 0	

2258. C₁₀H₁₆O

Neral

RN: 106-26-3

MP (°C):

MW: 152.24

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.898E-03	2.890E-01	25	L450	0 0 0 0 0	

2259. C₁₀H₁₆O₂

3-Hydroxy-3-ethynyl-2,2,5,5-tetramethyltetrahydrofuran

3-Furanol, 3-ethynyltetrahydro-2,2,5,5-tetramethyl-

RN: 24270-82-4 MP (°C):

MW: 168.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.165E-01	1.961E+01	rt	B066	0 2 0 0 0	

2260. C₁₀H₁₆O₃

cis-Pinonic acid

cis-3-Acetyl-2,2-dimethylcyclobutaneacetic acid

RN: 473-72-3 MP (°C): 104–107

MW: 184.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.001E-02	3.686E+00	0	H430	0 0 0 0 0	
3.612E-02	6.655E+00	rt	H431	0 0 0 0 0	average

2261. C₁₀H₁₆O₄

L-Isocamphoric acid

L-Isocamphersaeure

RN: 5394-83-2 MP (°C): 173

MW: 200.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.698E-02	3.400E+00	20	F300	1 0 0 0 1	

2262. C₁₀H₁₆O₄

D-Camphoric acid

D-Camphersaeure

RN: 124-83-4

MP (°C):

MW: 200.24

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.796E-02	7.600E+00	25	F300	1 0 0 0 1	

2263. C₁₀H₁₆O₅

DL-Cineolic acid

DL-Cineolsaeure

RN: 473-18-7

MP (°C): 208

MW: 216.24

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.474E-02	1.400E+01	15	F300	1 0 0 0 1	
3.006E-01	6.500E+01	100	F300	1 0 0 0 1	

2264. C₁₀H₁₇Cl₂NOS

Diallate

DATC

S-(2,3-Dichloroallyl)-N,N-diisopropylthiocarbamate

RN: 2303-16-4 MP (°C): -10

MW: 270.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-04	4.000E-02	25	B185	0 0 0 0 0	
5.181E-05	1.400E-02	25	B200	1 0 0 1 1	
1.480E-04	4.000E-02	25	M061	1 0 0 0 1	
5.181E-05	1.400E-02	25	M161	1 0 0 0 1	
1.480E-04	4.000E-02	ns	F019	0 0 0 0 1	
1.480E-04	4.000E-02	rt	I314	0 0 0 0 0	

2265. C₁₀H₁₇NO₂

Methyprylon

Dimerin

3,3-Diethyl-5-methyl-2,4-piperidinedione

RN: 125-64-4 MP (°C):

MW: 183.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.147E-01	7.600E+01	25	R027	0 0 0 0 0	

2266. C₁₀H₁₇N₂O₄PS

Etrimfos

Dimethyl *O*-(2-ethyl-4-ethoxy-pyrimidin-6-yl)thionophosphate

Ekamet G

Ekamet ULV

Etriphos

RN: 38260-54-7 **MP (°C):**
MW: 292.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.421E-02	1.000E+01	20	M161	1 0 0 0 1	
1.368E-04	3.998E-02	ns	S460	0 0 0 0 0	

2267. C₁₀H₁₇N₃O₅

Orotic acid choline

RN: **MP (°C):** 102–104
MW: 259.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.697E+00	6.992E+02	25	N018	0 0 0 0 0	

2268. C₁₀H₁₇N₃O₆S

Glutathione

Glutathion

RN: 70-18-8 **MP (°C):** 193.4
MW: 307.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.958E-01	9.090E+01	0	F300	1 0 0 0 2	

2269. C₁₀H₁₇O₃P

Diethyl phenyl phosphonate

Diethyl benzenephosphonate

Diethyl phenylphosphonate

RN: 1754-49-0 **MP (°C):**
MW: 216.22 **BP (°C):** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.25E-04	<2.00E-01	25	B070	1 2 0 1 0	

2270. C₁₀H₁₈

2,2,5,5-Tetramethyl-3-hexyne

Di-*tert*-butylacetyleneDi-*tert*-butylethyne

RN: 17530-24-4 MP (°C):

MW: 138.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-04	2.032E-02	25	H039	1 2 2 2 2	
7.700E-05	1.065E-02	35	H039	1 2 2 2 1	

2271. C₁₀H₁₈

Pinane

2,6,6-Trimethylbicyclo[3.1.1]heptane

2,7,7-Trimethylbicyclo[3.1.1]heptane

Dihydropinene

RN: 473-55-2 MP (°C):

MW: 138.25 BP (°C): 151

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-05	1.576E-03	ns	S460	0 0 0 0 0	

2272. C₁₀H₁₈

Decalin

Decahydronaphthalene

RN: 91-17-8 MP (°C): -31

MW: 138.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.45E-03	<2.00E-01	25	B019	1 0 1 2 0	
6.430E-06	8.890E-04	25	P051	2 1 1 2 2	
6.148E-06	8.500E-04	25	T423	0 0 0 0 0	
6.430E-06	8.890E-04	25.00	P007	2 1 2 2 2	
4.492E-05	6.210E-03	ns	H123	0 0 0 0 0	

2273. C₁₀H₁₈*cis*-Decalin*cis*-Decahydronaphthalene*cis*-Bicyclo[4.4.0]decane

RN: 493-01-6 MP (°C): -43.2

MW: 138.25 BP (°C): 195.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.452E-02	8.920E+00	300	S355	1 1 1 2 0	EFG

2274. C₁₀H₁₈ClN₅

Ipazine

2-Chloro-4-diethylamino-6-isopropylamino-s-triazine

2-Chloro-4-isopropylamino-6-diethylamino-s-triazines

RN: 1912-25-0 **MP (°C):****MW:** 243.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-04	4.000E-02	21	B192	0 0 0 0 1	
1.641E-04	4.000E-02	21	G099	2 0 0 1 0	
1.641E-04	4.000E-02	ns	B185	0 0 0 0 0	

2275. C₁₀H₁₈N₂O₄

Ethyl-2,2-diethylmalonurate

Ethyl 2,2-diethylmalonurate

RN: 73632-76-5 **MP (°C):** 84.5**MW:** 230.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-03	1.934E+00	23	B152	1 2 1 1 1	pH 3.5

2276. C₁₀H₁₈N₂O₅

Methoxymethyl-2,2-diethylmalonurate

Methoxymethyl 2,2-diethylmalonurate

RN: 73632-79-8 **MP (°C):** 113**MW:** 246.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	1.675E+00	23	B152	1 2 1 1 1	pH 3.5

2277. C₁₀H₁₈N₆O₂

1-(Sarcosino)-3,5-bis(dimethylamino)-s-triazine

N2-Carboxymethyl-N2,N4,N4,N6,N6-pentamethylmelamine

RN: 64124-17-0 **MP (°C):****MW:** 254.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.360E-02	1.872E+01	25	B386	0 0 0 0 0	

2278. C₁₀H₁₈O

Borneol

endo-1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol

L-Borneol

RN: 507-70-0 **MP (°C):** 206
MW: 154.25 **BP (°C):** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.512E-03	6.960E-01	15	M073	1 0 2 2 2	
4.784E-03	7.380E-01	25	M073	1 0 2 2 2	
4.786E-03	7.383E-01	ns	R427	0 0 0 0 0	

2279. C₁₀H₁₈O

D-Borneol

Borneocamphor

Sumatra camphor

endo-2-Bornanol

RN: 464-43-7 **MP (°C):** 208
MW: 154.25 **BP (°C):** 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.797E-03	7.400E-01	25	F300	1 0 0 0 1	

2280. C₁₀H₁₈O

L-Menthone

trans-p-Menthane-3-one*p*-Menthane-3-one

(-)-Methyl-2-(1-methylethyl)cyclohexanone

(-)-Menthone

RN: 14073-97-3 **MP (°C):** -6
MW: 154.25 **BP (°C):** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.220E-03	4.967E-01	25	I019	1 0 1 2 2	

2281. C₁₀H₁₈O

Linalool

3,7-Dimethylocta-1,6-dien-3-ol

2,6-Dimethylocta-2,7-dien-6-ol

Linalol

3,7-Dimethyl-1,6-octadien-3-ol

RN: 78-70-6 **MP (°C):** <25
MW: 154.25 **BP (°C):** 195.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-03	5.507E-01	6	P430	0 0 0 0 0	
5.530E-03	8.530E-01	23.5	P430	0 0 0 0 0	
1.200E-02	1.851E+00	25	D407	1 0 2 2 2	
1.030E-02	1.589E+00	25	I019	1 0 1 2 2	
9.710E-03	1.498E+00	25	M350	1 0 1 1 1	
3.800E-02	5.862E+00	37	E028	1 0 1 1 2	

2282. C₁₀H₁₈O

Citronellal

D-Citronellal

(R)-(+)-citronellal

3,7-Dimethyl-6-octen-1-al

3,7-Dimethyl-6-octenal

Rhodinal

RN: 106-23-0 **MP (°C):**
MW: 154.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	1.388E-01	25	A401	1 0 2 2 0	

2283. C₁₀H₁₈O

α-Terpineol

1-*p*-Menth-8-ol

1-Methyl-4-isopropyl-1-cyclohexen-8-ol

2-(4-Methyl-3-cyclohexenyl)-2-propanol

p-Menth-1-en-8-ol

α,α,4-Trimethyl-3-cyclohexene-1-methanol

RN: 98-55-5 **MP (°C):** 34.5
MW: 154.25 **BP (°C):** 218

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.202E-03	3.397E-01	6	P430	0 0 0 0 0	
4.600E-03	7.096E-01	23.5	P430	0 0 0 0 0	
1.620E-02	2.499E+00	25	A401	1 0 2 2 0	

2284. C₁₀H₁₈O

Nerol

Allerol

cis-3,7-Dimethyl-2,6-octadien-1-ol

Neraniol

Nerosol

Vernol

RN: 106-25-2 **MP (°C):**
MW: 154.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-03	1.311E+00	25	A401	1 0 2 2 0	

2285. C₁₀H₁₈O

Geraniol

2,6-Dimethyl-2,6-octadien-8-ol

2,6-Dimethyl-*trans*-2,6-octadien-8-ol2-*trans*-3,7-Dimethyl-2,6-octadiene-1-ol3,7-Dimethyl-*trans*-2,6-octadien-1-ol

(E)-3,7-Dimethyl-2,6-octadien-1-ol

RN: 106-24-1 **MP (°C):** 15
MW: 154.25 **BP (°C):** 229

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-03	7.713E-01	25	A401	1 0 2 2 0	

2286. C₁₀H₁₈O

Menthone

5-Methyl-2-(1-methylethyl)cyclohexanone

DL-Menthone

RN: 10458-14-7 **MP (°C):** -6
MW: 154.25 **BP (°C):** 207

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	3.085E-01	25	A401	1 0 2 2 0	

2287. C₁₀H₁₈O

Plinol

RN: 72402-00-7 **MP (°C):**
MW: 154.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.281E-03	8.146E-01	6	P430	0 0 0 0 0	
9.610E-03	1.482E+00	23.5	P430	0 0 0 0 0	

2288. C₁₀H₁₈O

1,8-Cineole

Eucalyptol

Cineol

Cineole

RN: 470-82-6**MP (°C):** 36.5**MW:** 154.25**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.123E-02	6.359E+00	1.5	E036	1 0 1 1 1	
4.187E-02	6.458E+00	4.0	B352	0 0 0 0 0	
3.674E-02	5.668E+00	7.5	E036	1 0 1 1 1	
3.482E-02	5.371E+00	10	E036	1 0 1 1 1	
3.610E-02	5.569E+00	10.0	B352	0 0 0 0 0	
1.297E-02	2.000E+00	15	F300	1 0 0 0 1	
3.097E-02	4.777E+00	15.0	B352	0 0 0 0 0	
2.261E-02	3.488E+00	21	E036	1 0 1 1 1	
2.454E-02	3.786E+00	21.0	B352	0 0 0 0 0	
2.010E-02	3.100E+00	25	A049	1 0 0 0 1	
2.197E-02	3.388E+00	25	B423	1 1 1 2 1	
1.746E-02	2.693E+00	30.0	B352	0 0 0 0 0	
1.552E-02	2.394E+00	35.0	B352	0 0 0 0 0	
9.100E-03	1.404E+00	37	E028	1 0 1 1 1	
1.359E-02	2.096E+00	40	E036	1 0 1 1 1	
1.423E-02	2.195E+00	40.0	B352	0 0 0 0 0	
1.294E-02	1.996E+00	45.0	B352	0 0 0 0 0	
1.229E-02	1.896E+00	50	E036	1 0 1 1 1	
1.100E-02	1.697E+00	50.0	B352	0 0 0 0 0	

2289. C₁₀H₁₈O₂

2,4-Decadione

Acetyl methyl hexyl ketone

RN: 13329-78-7 **MP (°C):****MW:** 170.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-03	4.427E-01	25	M078	2 0 1 0 1	

2290. C₁₀H₁₈O₂

3-Pentyl-2,4-pentadione

3-Amyl-2,4-pentanedi one

RN: 27970-50-9 **MP (°C):****MW:** 170.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-02	2.401E+00	25	M078	2 0 1 0 2	

2291. C₁₀H₁₈O₂

Sobrerol

Pinolhydrat

RN: 498-71-5

MP (°C): 130

MW: 170.25

BP (°C): 170

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-01	3.200E+01	15	F300	1 0 0 0 1	
1.938E-01	3.300E+01	ns	L335	0 0 0 0 2	

2292. C₁₀H₁₈O₂

D-Campholic acid

D-Campholsaeure

RN: 464-88-0

MP (°C):

MW: 170.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.398E-04	1.600E-01	19	F300	1 0 0 0 1	

2293. C₁₀H₁₈O₃

2,2,5,5-Tetramethyl-tetrahydro-3-hydroxy-3-furanyl methyl ketone

Ketone, methyl tetrahydro-3-hydroxy-2,2,5,5-tetramethyl-3-furyl

RN: 24282-51-7 MP (°C):

MW: 186.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.053E-01	1.961E+01	rt	B066	0 2 0 0 0	

2294. C₁₀H₁₈O₄

Sebacic acid

Sebacinsaeure

RN: 111-20-6 MP (°C): 134.5

MW: 202.25 BP (°C): 294.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.978E-04	4.000E-02	0	F300	1 0 0 0 0	
1.978E-04	4.000E-02	0	L041	1 0 0 1 0	
4.944E-03	1.000E+00	20	F300	1 0 0 0 1	
4.944E-03	1.000E+00	20	L041	1 0 0 1 1	
9.889E-03	2.000E+00	21	B040	1 0 1 1 1	<i>sic</i>
7.911E-03	1.600E+00	35	L041	1 0 0 1 1	
1.088E-02	2.200E+00	50	L041	1 0 0 1 1	
2.077E-02	4.200E+00	65	F300	1 0 0 0 1	
2.077E-02	4.200E+00	65	L041	1 0 0 1 1	
8.898E-04	1.800E-01	ns	F014	0 0 0 0 1	

2295. C₁₀H₁₈O₄

Amyl α-acetoxypropionate

Hydracrylic acid, pentyl ester, acetate

RN: 20473-77-2 MP (°C):

MW: 202.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.461E-03	7.000E-01	25	R006	2 2 0 1 1	

2296. C₁₀H₁₈O₄

Ethylene glycol dibutyrate

Ethylene glycol di-N-butylate

RN: 105-72-6 MP (°C):

MW: 202.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.220E-03	1.663E+00	25	F064	1 0 0 0 2	
2.471E-03	4.998E-01	ns	F014	0 0 0 0 1	

2297. C₁₀H₁₈O₄

Diethoxyethyl adipate

Diethyl adipate

RN: 141-28-6 MP (°C): -18

MW: 202.25 BP (°C): 251

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.965E-03	5.996E-01	ns	F014	0 0 0 0 1	
1.223E-02	2.474E+00	ns	F014	0 0 0 0 2	

2298. C₁₀H₁₈O₄

Dimethyl cyclohexyl oxalate

RN: MP (°C):

MW: 202.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.89E-06	<2.00E-03	15	H069	1 0 1 1 0	

2299. C₁₀H₁₈O₅

Diethylene glycol dipropionate

Ethanol, 2,2'-oxybis-, dipropionate

RN: 6942-59-2 MP (°C):

MW: 218.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.592E-01	3.475E+01	ns	F014	0 0 0 0 2	

2300. C₁₀H₁₈O₅

Propanoic acid, 2-[(ethoxycarbonyl)oxy]-, butyl ester
 Propanoic acid, 2-[(amoxycarbonyl)oxy]-, methyl ester

RN: MP (°C):
MW: 218.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.290E-03	4.998E-01	25	R007	0 0 0 0 0	
3.205E-03	6.995E-01	25	R007	0 0 0 0 0	

2301. C₁₀H₁₉NO₂S

4-Thiazolidinecarboxylic acid, 2-hexyl-
 Thiazolidine-4-carboxylic acid, 2-hexyl-

RN: 14347-74-1 **MP (°C):**
MW: 217.33 **BP (°C):** 378.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-03	6.085E-01	21	B414	1 0 0 1 1	partial decomposition

2302. C₁₀H₁₉NO₃

Ethylpropylaceturethane

RN: MP (°C):
MW: 201.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.088E-03	1.427E+00	c	O021	0 2 0 0 0	

2303. C₁₀H₁₉NO₃

Oenanthylurethane

RN: MP (°C):
MW: 201.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.043E-03	2.100E-01	ns	O021	0 0 0 0 0	

2304. C₁₀H₁₉NO₄S

2-Amino-5-naphthol-1-sulfonic acid

RN: MP (°C):
MW: 249.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.503E-03	2.120E+00	c	B125	1 2 0 0 2	

2305. C₁₀H₁₉N₂O₄PS

Cyanthroate

Phosphorothioic acid, *S*-(2-((1-cyano-1-methylethyl)amino)-2-oxoethyl) *O,O*-diethyl ester

Tartran

RN: 3734-95-0 **MP (°C):****MW:** 294.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.378E-01	7.000E+01	20	M161	1 0 0 0 1	

2306. C₁₀H₁₉N₅O

Prometone

2-Methoxy-4,6-*bis*-isopropylamino-*s*-triazine

Pramitol

Primatol O

Prometon

2-Methoxy-4,6-*bis*-(isopropyl-amino)-*s*-triazine**RN:** 1610-18-0 **MP (°C):** 91.5**MW:** 225.30 **BP (°C):** 91-92

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.330E-03	7.502E-01	20	B200	1 0 0 0 2	
2.752E-03	6.200E-01	20	F311	1 2 2 2 1	
3.329E-03	7.500E-01	20	M161	1 0 0 0 2	
3.329E-03	7.500E-01	21	B192	0 0 0 0 2	
1.554E-02	3.500E+00	21	G099	2 0 0 1 0	
3.329E-03	7.500E-01	21	G099	2 0 0 1 0	
4.680E-03	1.054E+00	50	G001	1 0 1 1 2	
3.548E-03	7.994E-01	ns	B100	0 0 0 0 0	
3.329E-03	7.500E-01	ns	B185	0 0 0 0 0	
3.329E-03	7.500E-01	ns	C101	0 0 0 0 1	
3.329E-03	7.500E-01	ns	G041	0 0 0 0 2	
3.329E-03	7.500E-01	ns	H112	0 0 0 0 2	
3.329E-03	7.500E-01	ns	J033	0 0 0 0 0	

2307. C₁₀H₁₉N₅O

Terebumeton

1,3,5-Triazine-2,4-diamine, *N*-(1,1-dimethylethyl)-*N'*-ethyl-6-methoxy-2-Methoxy-4-ethylamino-6-*tert*-butylamino-*s*-triazine

Karagard

4-(Ethylamino)-2-methoxy-6-(*tert*-butylamino)-*s*-triazine

Caragard

RN: 33693-04-8 **MP (°C):** 123.5**MW:** 225.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.770E-04	1.300E-01	20	M161	1 0 0 0 2	

2308. C₁₀H₁₉N₅O2-Methoxy-4-ethylamino-6-diethylamino-*s*-triazine

G 31432

RN: 13532-26-8 **MP (°C):**
MW: 225.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.775E-04	4.000E-02	20	J033	0 0 0 0 0	

2309. C₁₀H₁₉N₅O

Secbumeton

2-*sec*-Butylamino-4-ethylamino-6-methoxy-*s*-triazine

GS-14254

RN: 26259-45-0 **MP (°C):** 86
MW: 225.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.930E-03	6.601E-01	1	G091	1 0 1 2 2	pH 6.0
3.250E-03	7.322E-01	8	G091	1 0 1 2 2	pH 6.0
2.750E-03	6.196E-01	20	B200	1 0 0 0 2	
2.663E-03	6.000E-01	20	F311	1 2 2 2 1	
3.070E-03	6.917E-01	20	G091	1 0 1 2 2	pH 6.0
2.752E-03	6.200E-01	20	M161	1 0 0 0 2	
3.300E-03	7.435E-01	29	G091	1 0 1 2 2	pH 6.0

2310. C₁₀H₁₉N₅OS

Hydroxyprometryne

1,3,5-Triazin-2(1H)-one, 4,6-bis[(1-methylethyl)amino]-
bis(Isopropylamino)hydroxy-*s*-triazine

GS 11526

RN: 7374-53-0 **MP (°C):**
MW: 257.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	1.029E-01	2	B193	1 2 0 0 0	

2311. C₁₀H₁₉N₅S

Terbutryn

2-Methylthio-4-ethylamino-6-*tert*-butylamino-*s*-triazine

Terbutryne

N-(1,1-Dimethylethyl)-N'-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine

Terbutrex

RN: 886-50-0 **MP (°C):** 104
MW: 241.36 **BP (°C):** 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-04	2.631E-02	1	G091	1 0 1 2 2	pH 6.0
1.100E-04	2.655E-02	8	G091	1 0 1 2 2	pH 6.0
2.400E-04	5.793E-02	20	B200	1 0 0 0 1	
1.036E-04	2.500E-02	20	E048	1 2 1 1 1	
1.036E-04	2.500E-02	20	F311	1 2 2 2 1	
1.460E-04	3.524E-02	20	G091	1 0 1 2 2	pH 6.0
2.403E-04	5.800E-02	20	M161	1 0 0 0 1	
1.660E-04	4.007E-02	29	G091	1 0 1 2 2	pH 6.0
2.403E-04	5.800E-02	ns	J033	0 0 0 0 0	

2312. C₁₀H₁₉N₅S

Prometryne

N,N'-bis(1-Methylethyl)-6-methylthio-1,3,5-triazine-2,4-diamine

Caparol

Primatol Q

Gesagard

Caparol 80W

RN: 7287-19-6 **MP (°C):** 118
MW: 241.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	5.793E-02	2	B193	1 2 0 0 0	
2.000E-04	4.827E-02	20	B200	1 0 0 0 0	
1.657E-04	4.000E-02	20	F311	1 2 2 2 1	
1.988E-03	4.798E-01	20	M061	1 0 0 0 1	
1.989E-04	4.800E-02	20	M161	1 0 0 0 1	
1.989E-04	4.800E-02	24	C105	2 1 2 2 2	
4.200E-04	1.014E-01	50	G001	1 0 1 1 2	
1.989E-04	4.800E-02	ns	C101	0 0 0 0 1	
1.989E-04	4.800E-02	ns	H112	0 0 0 0 1	
1.989E-04	4.800E-02	ns	J033	0 0 0 0 0	

2313. C₁₀H₁₉N₅S

s-Triazole, 2,4-bis(isopropylamine)-6-methylmercapto-

RN: MP (°C):

MW: 241.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.989E-04	4.800E-02	20	B185	0 0 0 0 0	

2314. C₁₀H₁₉O₆PS₂

Malathion

Dicarboethoxyethyl O,O-dimethyl phosphorodithioate

Carbofos

Cythion

Mercaptothion

Phosphothion

RN: 121-75-5 MP (°C): 3

MW: 330.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.267E-04	1.410E-01	10	B324	0 0 0 0 0	
4.268E-04	1.410E-01	10	B324	0 0 0 0 0	
4.329E-04	1.430E-01	20	B300	2 1 1 1 2	
4.389E-04	1.450E-01	20	B324	0 0 0 0 0	
4.388E-04	1.450E-01	20	B324	0 0 0 0 0	
4.389E-04	1.450E-01	20	F311	1 2 2 2 1	
4.389E-04	1.450E-01	20	M061	1 0 0 0 2	
4.389E-04	1.450E-01	20	M344	1 0 0 0 2	
4.964E-04	1.640E-01	30	B324	0 0 0 0 0	
4.963E-04	1.640E-01	30	B324	0 0 0 0 0	
4.389E-04	1.450E-01	rt	M161	0 0 0 0 2	

2315. C₁₀H₂₀

Cyclodecane

RN: 293-96-9 MP (°C): 10

MW: 140.27 BP (°C): 202

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.353E-06	3.300E-04	25	T423	0 0 0 0 0	

2316. C₁₀H₂₀*n*-Pentylcyclopentane

1-Pentylcyclopentane

RN: 3741-00-2 MP (°C):

MW: 140.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.198E-07	1.150E-04	25	K119	1 0 0 0 2	
8.198E-07	1.150E-04	25	P051	2 1 1 2 2	
8.198E-07	1.150E-04	25.00	P007	2 1 2 2 2	

2317. C₁₀H₂₀NO₄PS

Propetamphos

Methylethyl (E)-3-(((ethylamino)methoxyphosphinothioyl)oxy)-2-butenoate

Safrotin

Seraphos

Zoecon

RN: 31218-83-4 MP (°C):

MW: 281.31 BP (°C): 88

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.910E-04	1.100E-01	24	M161	1 0 0 0 2	

2318. C₁₀H₂₀NO₅PS₂

Mecarbam

O,O-Diethyl *S*-(*N*-methyl-*N*-carboethoxycarbamoylmethyl) dithiophosphate

RN: 2595-54-2 MP (°C):

MW: 329.38 BP (°C): 144

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.033E-03	9.990E-01	rt	M061	0 0 0 0 0	
<3.04E-03	<1.00E+00	rt	M161	0 0 0 0 0	

2319. C₁₀H₂₀N₂S₄

Disulfiram

Tetraethylthioperoxydicarbonothioic diamide

Tetraethylthiuram disulfide

Antadix

Antabuse

Esperal

RN: 97-77-8 MP (°C): 70

MW: 296.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.744E-04	2.000E-01	25	I314	0 0 0 0 0	
1.379E-05	4.090E-03	25	L033	1 0 2 1 2	<i>sic</i>
1.012E-03	3.000E-01	ns	N061	0 0 0 0 0	

2320. C₁₀H₂₀N₆O

N-(Methoxymethyl)pentamethylmelamine
N-Methylolpentamethylmelamine methyl ether
 RN: 64124-15-8 MP (°C): 39
 MW: 240.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-03	1.500E+00	25	C051	1 2 1 1 1	pH 7, unstable in water

2321. C₁₀H₂₀O

Citronellol
 3,7-Dimethyl-6-octen-1-ol
 Levo-citronellol
 β-Citronellol
 RN: 106-22-9 MP (°C):
 MW: 156.27 BP (°C): 222

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-03	2.000E-01	25	M350	1 0 1 1 1	

2322. C₁₀H₂₀O

Decanal
 Cuprylaldehyde
 RN: 112-31-2 MP (°C): 7
 MW: 156.27 BP (°C): 207–209

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.983E-05	1.560E-02	25	L450	0 0 0 0 0	

2323. C₁₀H₂₀O

Menthol
 Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1α,2β,5α)-
 3-*p*-Menthanol
 RN: 89-78-1 MP (°C): 42
 MW: 156.27 BP (°C): 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-03	4.000E-01	20	F300	1 0 0 0 2	
2.920E-03	4.563E-01	25	I019	1 0 1 2 2	
8.600E-03	1.344E+00	37	E028	1 0 1 1 1	

2324. C₁₀H₂₀O

l-Menthol

1-Isopropyl-4-methyl cyclohexan-2-ol

1-Methyl-4-isopropyl cyclohexan-3-ol

(1R,2S,5R)-(-)-Menthol

5-Methyl-2-isopropyl hexahydrophenol

Cyclohexanol

RN: 2216-51-5 MP (°C): 44

MW: 156.27 BP (°C): 212

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	6.251E-01	25	A401	1 0 2 2 0	

2325. C₁₀H₂₀O₂

3-Hydroxy-2-ethyl-5-propyl-5-methyltetrahydrofuran

3-Furanol, 2-ethyltetrahydro-5-methyl-5-propyl-

RN: 29839-73-4 MP (°C):

MW: 172.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2326. C₁₀H₂₀O₂

3-Hydroxy-2,2-dimethyl-5,5-diethyltetrahydrofuran

3-Furanol, 5,5-diethyltetrahydro-2,2-dimethyl-

RN: 29839-77-8 MP (°C):

MW: 172.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-02	4.975E+00	rt	B066	0 2 0 0 0	

2327. C₁₀H₂₀O₂

3-Hydroxy-2,5,5-triethyltetrahydrofuran

3-Furanol, 2,5,5-triethyltetrahydro-

RN: 29839-70-1 MP (°C):

MW: 172.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2328. C₁₀H₂₀O₂

3-Hydroxy-2,5-dipropyltetrahydrofuran

3-Furanol, 2,5-dipropyltetrahydro-

RN: 30003-27-1 **MP (°C):****MW:** 172.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	rt	B066	0 2 0 0 0	

2329. C₁₀H₂₀O₂

3-Hydroxy-2-butyl-5,5-methyltetrahydrofuran

3-Furanol, 2-butyltetrahydro-5,5-dimethyl-

RN: 29839-71-2 **MP (°C):****MW:** 172.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.888E-02	4.975E+00	rt	B066	0 2 0 0 0	

2330. C₁₀H₂₀O₂

3-Hydroxy-2-pentyl-5-methyltetrahydrofuran

3-Furanol, 5-methyltetrahydro-2-pentyl-

RN: 29848-45-1 **MP (°C):****MW:** 172.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.159E-02	1.996E+00	rt	B066	0 2 0 0 0	

2331. C₁₀H₂₀O₂

3-Hydroxy-2-propyl-5-methyl-5-ethyltetrahydrofuran

3-Furanol, 5-ethyltetrahydro-5-methyl-2-propyl-

RN: 29839-72-3 **MP (°C):****MW:** 172.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2332. C₁₀H₂₀O₂*n*-Capric acid

Caprinsaeure

Decanoic acid

Nonanecarboxylic acid

RN: 334-48-5

MP (°C): 31.4

MW: 172.27

BP (°C): 270

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.515E-04	9.500E-02	0	B136	1 0 2 1 1	
1.509E-04	2.600E-02	15	F300	1 0 0 0 1	
2.902E-04	5.000E-02	20	A011	1 2 1 1 1	
9.462E-04	1.630E-01	20	B136	1 0 2 1 2	
8.706E-04	1.500E-01	20	D041	1 0 0 0 1	
8.706E-04	1.500E-01	20.0	R001	1 1 1 1 1	
3.590E-04	6.184E-02	25	J001	1 0 2 1 2	
1.115E-03	1.920E-01	30	B136	1 0 2 1 2	
3.715E-04	6.400E-02	30	E005	2 1 1 2 1	
1.045E-03	1.800E-01	30.0	R001	1 1 1 1 1	
1.294E-03	2.230E-01	40	B136	1 0 2 1 2	
4.179E-04	7.200E-02	40	E005	2 1 1 2 1	
1.335E-03	2.300E-01	45	B136	1 0 2 1 1	
1.335E-03	2.299E-01	45.0	R001	1 1 1 1 1	
4.702E-04	8.100E-02	50	E005	2 1 1 2 1	
5.000E-04	8.613E-02	50	J001	1 0 2 1 2	
1.567E-03	2.700E-01	60	B136	1 0 2 1 1	
5.805E-04	1.000E-01	60	E005	2 1 1 2 2	
1.567E-03	2.699E-01	60.0	R001	1 1 1 1 1	
5.514E-04	9.499E-02	.0	R001	1 1 1 1 1	

2333. C₁₀H₂₀O₂

3-Hydroxy-5,5-dipropyltetrahydrofuran

3-Furanol, 5,5-dipropyltetrahydro-

RN: 29839-54-1 MP (°C):

MW: 172.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2334. C₁₀H₂₀O₂

3-Hydroxy-5,5-diisopropyltetrahydrofuran

3-Furanol, 5,5-diisopropyltetrahydro-

RN: 29839-55-2 MP (°C):

MW: 172.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.747E-02	9.901E+00	rt	B066	0 2 0 0 0	

2335. C₁₀H₂₀O₂

3-Hydroxy-2,5-dimethyl-2,5-diethyltetrahydrofuran
3-Furanol, 2,5-diethyltetrahydro-2,5-dimethyl-

RN: 30010-09-4 **MP (°C):**
MW: 172.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-01	1.961E+01	rt	B066	0 2 0 0 0	

2336. C₁₀H₂₀O₂·H₂O

Terpin (monohydrate)
Terpin-hydrat

RN: 2451-01-6 **MP (°C):** 116
MW: 190.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.102E-02	4.000E+00	15	F300	1 0 0 0 0	
1.799E-02	3.424E+00	25	M012	1 0 2 1 2	
1.661E-01	3.160E+01	100	F300	1 0 0 0 2	

2337. C₁₀H₂₀O₃

1,3-Dioxolane-4-methanol, 2-methyl-2-pentyl
2-Heptanone, cyclic (hydroxymethyl)ethylene acetal
2-Methyl-2-*n*-amyl-4-hydroxymethyl-1,3-dioxolane
2-Methyl-2-pentyl-1,3-dioxolane-4-methanol

RN: 4361-59-5 **MP (°C):**
MW: 188.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.090E-02	9.583E+00	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

2338. C₁₀H₂₀O₃

n-Amyl β-ethoxypropionate
Propionic acid, 3-ethoxy-, pentyl ester
RN: 14144-36-6 **MP (°C):**
MW: 188.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.366E-03	1.199E+00	25	D002	1 2 1 1 1	

2339. C₁₀H₂₀O₄

Butyl carbitol acetate

Diethylene glycol acetate butyl ether

Diethylene glycol butyl ether acetate

Diglykol-monobutylaether-acetat

RN: 124-17-4 MP (°C): -32

MW: 204.27 BP (°C): 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.709E-02	1.575E+01	20	D052	1 1 0 0 1	
1.792E-01	3.661E+01	20	M062	1 0 0 0 1	

2340. C₁₀H₂₁NOS

Pebulate

S-Propyl butylethylthiocarbamate

RN: 1114-71-2 MP (°C): <25

MW: 203.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.951E-04	6.000E-02	20	M161	1 0 0 0 1	
4.524E-04	9.200E-02	21	F019	1 0 0 0 1	
4.524E-04	9.200E-02	21	M061	1 0 0 0 1	
2.951E-04	6.000E-02	ns	B200	0 0 0 0 1	
2.951E-04	6.001E-02	ns	S460	0 0 0 0 0	

2341. C₁₀H₂₁NOS

Vernolate

S-Propyl dipropylthiocarbamate

Carbamic acid, dipropylthio-, S-propyl ester

Carbamate, *n*-propyl-di-*n*-propylthio-

Vernam

RN: 1929-77-7 MP (°C): <25

MW: 203.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.426E-04	9.000E-02	20	B200	1 0 0 0 1	
5.262E-04	1.070E-01	21	F019	1 0 0 0 2	
5.262E-04	1.070E-01	21	M161	1 0 0 0 2	
<4.92E-04	<1.00E-01	ns	B185	0 0 0 0 0	
4.917E-04	9.999E-02	ns	M061	0 0 0 0 0	

2342. C₁₀H₂₂

2,2-Dimethyloctane

RN: 15869-87-1

MP (°C):

MW: 142.29

BP (°C): 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.499E-07	1.067E-04	ns	S460	0 0 0 0 0	

2343. C₁₀H₂₂*n*-Decane

Decane

Decyl hydride

RN: 124-18-5

MP (°C): -30.0

MW: 142.29

BP (°C): 174.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-07	1.976E-05	20	B165	1 0 1 1 1	
1.124E-07	1.600E-05	25	B069	1 0 1 1 1	
1.389E-07	1.976E-05	25	F004	0 0 0 0 0	
3.655E-07	5.200E-05	25	M003	1 0 2 2 1	
3.655E-07	5.200E-05	25	M040	1 0 0 1 1	
3.233E-07	4.600E-05	25	T423	0 0 0 0 0	
1.546E-07	2.200E-05	ns	B033	0 0 0 0 2	
1.546E-07	2.200E-05	ns	B033	0 0 0 0 0	
3.655E-07	5.200E-05	ns	H123	0 0 0 0 0	

2344. C₁₀H₂₂

4,4-Dimethyloctane

RN: 15869-95-1

MP (°C):

MW: 142.29

BP (°C): 157.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.546E-05	2.200E-03	20	M337	2 1 2 2 1	
7.278E-07	1.036E-04	ns	S460	0 0 0 0 0	

2345. C₁₀H₂₂

2,3-Dimethyloctane

RN: 7146-60-3

MP (°C):

MW: 142.29

BP (°C): 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.117E-07	7.281E-05	ns	S460	0 0 0 0 0	

2346. C₁₀H₂₂

2,6-Dimethyloctane

RN: 2051-30-1

MP (°C):

MW: 142.29

BP (°C): 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.266E-07	8.916E-05	ns	S460	0 0 0 0 0	

2347. C₁₀H₂₂

3,6-Dimethyloctane

RN: 15869-94-0

MP (°C):

MW: 142.29

BP (°C): 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.109E-07	8.693E-05	ns	S460	0 0 0 0 0	

2348. C₁₀H₂₂

3-Ethyloctane

RN: 5881-17-4

MP (°C):

MW: 142.29

BP (°C): 167

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.581E-07	6.519E-05	ns	S460	0 0 0 0 0	

2349. C₁₀H₂₂

4-Methylnonane

4-Methylnonane(DL)

RN: 17301-94-9

MP (°C):

MW: 142.29

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.764E-07	6.779E-05	ns	S460	0 0 0 0 0	

2350. C₁₀H₂₂

3,3-Dimethyloctane

RN: 4110-44-5

MP (°C):

MW: 142.29

BP (°C): 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.998E-07	8.534E-05	ns	S460	0 0 0 0 0	

2351. C₁₀H₂₂

4-Ethyloctane

RN: 15869-86-0 **MP (°C):**
MW: 142.29 **BP (°C):** 164

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.297E-07	7.536E-05	ns	S460	0 0 0 0 0	

2352. C₁₀H₂₂

3,5-Dimethyloctane

RN: 15869-93-9 **MP (°C):**
MW: 142.29 **BP (°C):** 159

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.546E-07	9.315E-05	ns	S460	0 0 0 0 0	

2353. C₁₀H₂₂

3-Methylnonane

3-Methylnonane(DL)

RN: 5911-04-6 **MP (°C):**
MW: 142.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.295E-07	6.112E-05	ns	S460	0 0 0 0 0	

2354. C₁₀H₂₂O

Decanol

RN: 36729-58-5 **MP (°C):**
MW: 158.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	3.166E-02	24	H345	0 0 0 0 0	

2355. C₁₀H₂₂O*n*-Decyl alcohol

Alcohol C-10

Nonyl acarbinol

Capric alcohol

RN: 36729-58-5 **MP (°C):****MW:** 158.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	4.258E-02	20	H330	0 0 0 0 0	
2.000E-04	3.166E-02	24	H345	2 0 2 2 2	
2.340E-04	3.704E-02	25	K025	2 2 1 1 2	
2.527E-05	4.000E-03	40	W305	1 0 0 1 0	EFG
3.000E-04	4.748E-02	ns	H012	0 2 2 0 0	

2356. C₁₀H₂₃O₂PS₂

Cadusafos

Ebufos

Taredan

Rugby

Apache

O-ethyl *S,S*-bis(1-methylpropyl) phosphorodithioate**RN:** 95465-99-9 **MP (°C):****MW:** 270.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.162E-04	2.477E-01	ns	S460	0 0 0 0 0	

2357. C₁₀H₂₃O₃P

Ethyl dibutyl phosphonate

Dibutyl ethyl phosphonate

RN: 2404-58-2 **MP (°C):****MW:** 222.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.699E-02	6.000E+00	25	B070	1 2 0 1 0	
5.849E-02	1.300E+01	25	B070	1 2 0 1 1	

2358. C₁₀H₂₃O₄P

Dibutyl ethyl phosphate

RN: 7242-58-2 **MP (°C):****MW:** 238.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.427E-02	3.400E+00	25	B070	1 2 2 1 1	

2359. C₁₀Cl₁₀O

Chlordecone

Kepone

1,2,3,5,6,7,8,9,10,10-Decachloropentacyclo[5.2.1.0(2,6).0(3,9).0(5,8)]decano-4-one

Merex

Decachloroketone

RN: 143-50-0 **MP (°C):**
MW: 490.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.153E-03	4.000E+00	100	M161	1 0 0 0 0	
6.166E-06	3.025E-03	ns	R424	0 0 0 0 0	
6.166E-06	3.025E-03	ns	R427	0 0 0 0 0	

2360. C₁₀Cl₁₂

Mirex

1,2,3,4,5,5-Hexachloro-1,3-cyclopentadiene dimer

Bichlorendo

Ferriamicide

Dechlorane 4070

RN: 2385-85-5 **MP (°C):**
MW: 545.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.549E-07	8.450E-05	24.99	K436	0 0 0 0 0	
1.397E-10	7.619E-08	25	H434	0 0 0 0 0	
1.558E-07	8.500E-05	25	M134	1 2 1 1 1	
1.741E-07	9.500E-05	ns	M110	0 0 0 0 0	EFG
1.660E-07	9.054E-05	ns	R427	0 0 0 0 0	

2361. C₁₁H₆BrNS

1-Bromo-2-naphthylisothiocyanate

RN: 2392-80-5 **MP (°C):**
MW: 264.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-05	1.268E-02	25	D019	1 1 1 1 1	

2362. C₁₁H₆O₃

Psoralen

7H-Furo[3,2-g][1]benzopyran-7-one

RN: 66-97-7 **MP (°C):** 158–161
MW: 186.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-04	6.516E-02	25	A355	0 0 0 0 0	

2363. C₁₁H₇Cl₂NO₃

Pyoluteorin

RN:**MW:** 272.09**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-04	1.442E-01	5.0	L451	0 0 0 0 0	
5.600E-04	1.524E-01	10	L451	0 0 0 0 0	
6.300E-04	1.714E-01	15.0	L451	0 0 0 0 0	
7.500E-04	2.041E-01	20.0	L451	0 0 0 0 0	
7.900E-04	2.150E-01	25.0	L451	0 0 0 0 0	
9.600E-04	2.612E-01	30.0	L451	0 0 0 0 0	
9.900E-04	2.694E-01	35.0	L451	0 0 0 0 0	
1.150E-03	3.129E-01	40.0	L451	0 0 0 0 0	
1.290E-03	3.510E-01	45.0	L451	0 0 0 0 0	
1.500E-03	4.081E-01	50.0	L451	0 0 0 0 0	
1.590E-03	4.326E-01	55.0	L451	0 0 0 0 0	
1.730E-03	4.707E-01	60.0	L451	0 0 0 0 0	

2364. C₁₁H₇FN₂O₃

3-Benzoyl-5-fluorouracil

RN: 61251-77-2**MP (°C):** 169–170**MW:** 234.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.551E-03	1.300E+00	22	B321	0 0 0 0 0	pH 4.0
5.551E-03	1.300E+00	22	B332	1 1 0 0 1	pH 4.0

2365. C₁₁H₇FN₂O₄

3-Phenoxy carbonyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

3-Phenoxy carbonyl-5-fluorouracil

RN: 66999-97-1**MP (°C):** 169–170**MW:** 250.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.995E-04	1.500E-01	22	B321	0 0 0 0 0	pH 4.0

2366. C₁₁H₇FN₂O₄

1-Phenoxy carbonyl-5-fluorouracil

RN: 75410-28-5**MP (°C):****MW:** 250.19**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.597E-03	9.000E-01	22	B332	1 1 0 0 1	pH 4.0

2367. C₁₁H₇NS

2-Naphthyl isothiocyanate
 2-Isothiocyanatonaphthalene
 β-Naphthyl mustard oil

RN: 1636-33-5 **MP (°C):**
MW: 185.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-05	6.669E-03	25	D019	1 1 1 1 1	

2368. C₁₁H₇NS

1-Naphthyl isothiocyanate
 1-Isothiocyanatonaphthalene
 α-Naphthyl mustard oil
 Kesscocide

ANI
 ANIT
RN: 551-06-4 **MP (°C):** 58.0
MW: 185.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	4.631E-03	25	D019	1 1 1 1 1	

2369. C₁₁H₈N₂

β-Carboline
 β-Carbolin
 Norharmane
 9H-Pyrido(3,4-b)indole

RN: 244-63-3 **MP (°C):** 199
MW: 168.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.391E+01	2.340E+03	16	B413	1 0 2 2 1	
1.601E+01	2.693E+03	17	B413	1 0 2 2 1	
2.535E+01	4.264E+03	37	B413	1 0 2 2 1	
2.561E+01	4.308E+03	38	B413	1 0 2 2 1	
2.916E+01	4.905E+03	45	B413	1 0 2 2 1	

2370. C₁₁H₈N₄O₄

Orotic acid nicotinamide

RN: **MP (°C):** 252–253
MW: 260.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-02	1.769E+01	25	N018	0 0 0 0 0	

2371. C₁₁H₈O₂

2-Naphthoic acid

 β -Naphthoic acid

2-Naphthalenecarboxylic acid

RN: 93-09-4 **MP (°C):****MW:** 172.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	2.238E-02	25	M149	2 2 2 2 1	intrinsic, <i>sic</i>
1.617E-06	2.785E-04	30	K148	1 1 0 0 2	
2.323E-06	4.000E-04	40	K148	1 1 0 0 1	
3.165E-06	5.450E-04	50	K148	1 1 0 0 2	
3.949E-06	6.800E-04	60	K148	1 1 0 0 2	
4.652E-06	8.010E-04	70	K148	1 1 0 0 2	
5.459E-06	9.400E-04	80	K148	1 1 0 0 2	
6.261E-06	1.078E-03	90	K148	1 1 0 0 2	

2372. C₁₁H₈O₂

Menadione

2-Methyl-1,4-naphthoquinone

Vitamin K3

Kativ-G

Panosine

Menaphthone

RN: 58-27-5 **MP (°C):** 106**MW:** 172.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.291E-04	1.600E-01	25	P096	0 0 0 0 0	
6.969E-04	1.200E-01	30	K090	1 2 2 2 0	EFG
8.700E-04	1.498E-01	30	O321	0 0 0 0 0	
8.710E-04	1.500E-01	30	O321	0 0 0 0 0	
9.291E-04	1.600E-01	30.00	E033	1 0 2 1 0	EFG
8.888E-04	1.530E-01	33	D404	2 1 2 2 2	
8.768E-04	1.510E-01	33	D404	2 1 2 2 2	
1.161E-03	2.000E-01	37.00	E033	1 0 2 1 0	EFG

2373. C₁₁H₈O₃

8-Hydroxypsoralon

RN: **MP (°C):****MW:** 188.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-04	1.148E-01	25	A355	0 0 0 0 0	

2374. C₁₁H₈O₃

2-Methoxy-1,4-naphthoquinone
 1,4-Naphthalenedione, 2-methoxy-
 2-Methoxy-1,4-naphthoquinone

RN: 2348-82-5 **MP (°C):**
MW: 188.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-04	3.123E-02	ns	R427	0 0 0 0 0	

2375. C₁₁H₉ClO₂S

Tianafac

RN: 51527-19-6 **MP (°C):**
MW: 240.71 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.444E-04	3.476E-02	25	C314	0 0 0 0 0	
1.442E-04	3.470E-02	25	C314	0 0 0 0 0	

2376. C₁₁H₉Cl₂NO₂

Barban

4-Chloro-2-butynyl-*N*-(3-chlorophenyl)carbamate4-Chloro-2-butynyl-*m*-chlorocarbonilate

RN: 101-27-9 **MP (°C):** 75
MW: 258.11 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.262E-05	1.100E-02	25	B200	1 0 0 0 2	
4.262E-05	1.100E-02	25	M161	1 0 0 0 1	
3.874E-05	1.000E-02	ns	H042	0 0 0 0 1	
4.262E-04	1.100E-01	ns	M061	0 0 0 0 2	

2377. C₁₁H₉Cl₄NO₄

OCS-21693

TMMT

Methyl-2,3,5,6-tetrachloro-*N*-methoxy-*N*-methylterephthalamate

RN: 14419-01-3 **MP (°C):** 96
MW: 361.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.385E-05	5.000E-03	25	B200	1 0 0 0 0	

2378. C₁₁H₉I₃N₂O₄

3,5-Diacetylaminoo-2,4,6-triiodobenzoic acid

Iothalamic acid

Diatrazoic acid

RN: 117-96-4**MP (°C):****MW:** 613.92**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.144E-01	5.000E+02	25	L100	1 0 0 0 2	
9.773E-01	6.000E+02	50	L100	1 0 0 0 2	
1.189E+00	7.297E+02	90	L100	1 0 0 0 2	
2.557E-03	1.570E+00	ns	H055	0 0 0 0 0	

2379. C₁₁H₁₀

2-Methylnaphthalene

2-Methyl naphthalene

β-Methyl naphthalenes

RN: 91-57-6**MP (°C):** 35**MW:** 142.20**BP (°C):** 241.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E-04	2.460E-02	25	E004	2 1 2 2 2	
1.828E-04	2.600E-02	25	L332	1 1 1 1 0	
1.786E-04	2.540E-02	25	M064	1 1 2 2 2	
1.800E-04	2.560E-02	25	M342	1 0 1 1 1	
1.758E-04	2.500E-02	25	O320	0 0 0 0 0	
1.786E-04	2.540E-02	ns	H123	0 0 0 0 0	
8.000E-05	1.138E-02	ns	L060	0 0 0 0 0	
1.786E-04	2.540E-02	ns	M344	0 0 0 0 2	

2380. C₁₁H₁₀

1-Methylnaphthalene

1-Methyl naphthalene

1-Methyl-naphthalene

α-Methyl naphthalenes

α-Methylnaphthalene

RN: 90-12-0**MP (°C):** -22**MW:** 142.20**BP (°C):** 244

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.739E-04	2.473E-02	4	D351	1 2 1 1 2	
1.600E-04	2.275E-02	10	S076	2 2 2 2 1	
2.000E-04	2.844E-02	14	S076	2 2 2 2 1	
1.195E-04	1.700E-02	20	A050	1 0 1 1 1	
2.145E-04	3.050E-02	20	B318	0 0 0 0 0	EFG
2.124E-04	3.020E-02	20	B356	0 0 0 0 0	
2.000E-04	2.844E-02	20	S076	2 2 2 2 1	
2.100E-04	2.986E-02	21	A057	2 1 2 2 1	

(continued)

2380. C₁₁H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.489E-04	3.539E-02	25	D351	1 2 1 1 2	
1.814E-04	2.580E-02	25	E004	2 1 2 2 2	
1.899E-04	2.700E-02	25	L332	1 1 2 1 0	
2.004E-04	2.850E-02	25	M064	1 1 2 2 2	
2.000E-04	2.844E-02	25	M342	1 0 1 1 2	
2.100E-04	2.986E-02	25	S076	2 2 2 2 1	
2.440E-04	3.470E-02	28	B348	2 2 2 2 2	
2.955E-04	4.203E-02	40	D351	1 2 1 1 2	
2.004E-04	2.850E-02	ns	H123	0 0 0 0 0	
1.600E-04	2.275E-02	ns	L060	0 0 0 0 1	
2.004E-04	2.850E-02	ns	M344	0 0 0 0 2	

2381. C₁₁H₁₀BrN₃O₂S

5-Sulfanilamido-2-bromopyridine

Benzenesulfonamide, 4-amino-N-(2-bromo-5-pyridinyl)-

RN: 17103-43-4 MP (°C):

MW: 328.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.717E-04	1.220E-01	37	R058	1 2 1 1 2	

2382. C₁₁H₁₀BrN₃O₂S

2-Sulfanilamido-5-bromopyridine

Benzenesulfonamide, 4-amino-N-(5-bromo-2-pyridinyl)-

RN: 16805-99-5 MP (°C):

MW: 328.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.158E-04	3.800E-02	37	R058	1 2 1 1 1	

2383. C₁₁H₁₀ClNO₂

Chlorbupham

1-Methylpropyn-2-yl N-(*m*-chlorophenyl)carbamate

Chlorbufam

Bi-PC

RN: 1967-16-4 MP (°C): 45.5

MW: 223.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.414E-03	5.400E-01	20	B185	0 0 0 0 0	
2.414E-03	5.400E-01	20	M161	1 0 0 0 2	

2384. C₁₁H₁₀ClN₃O₂S

5-Sulfanilamido-2-chloropyridine

N1-(6-Chloro-3-pyridyl)sulfanilamide

RN: 34392-82-0 MP (°C):

MW: 283.74 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.344E-04	1.800E-01	37	R058	1 2 1 1 1	

2385. C₁₁H₁₀Cl₂O₃

2,4-Dichlorophenoxyacetic acid allyl ester

Allyl 2,4-dichlorophenoxyacetate

RN: 58965-05-2 MP (°C):

MW: 261.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	3.722E-02	ns	M120	0 0 1 1 2	

2386. C₁₁H₁₀IN₃O₂S

2-Sulfanilamido-5-iodopyridine

Benzenesulfonamide, 4-amino-N-(5-iodo-2-pyridinyl)-

RN: 71119-21-6 MP (°C):

MW: 375.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.465E-05	1.300E-02	37	R058	1 2 1 1 1	

2387. C₁₁H₁₀N₂O3-*o*-Toluoxyypyridazine

Credazine

3-(2-Methylphenoxy)-pyridazine

RN: 14491-59-9 MP (°C): 78

MW: 186.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-02	1.996E+00	ns	B100	0 0 0 0 0	
1.074E-02	2.000E+00	rt	M161	0 0 0 0 0	

2388. C₁₁H₁₀N₂O

Vasicinone

Pyrrolo[2,1-b]quinazolin-9(1H)-one, 2,3-dihydro-3-hydroxy-, (3*S*)-

(-)-Vasicinone

L-Vasicinone

RN: 486-64-6 MP (°C): 204

MW: 186.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.578E-03	1.597E+00	25	B194	2 2 2 2 1	

2389. C₁₁H₁₀N₂O₃

Phenylmethylbarbituric acid

Barbituric acid, 5-methyl-5-phenyl

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-methyl-5-phenyl

2,4,6-Trioxo-5-methyl-5-phenylhexahydropyrimidine

Heptobarbital

RN: 76-94-8 MP (°C): 226

MW: 218.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-03	7.594E-01	20	J030	1 2 2 2 1	
4.170E-03	9.100E-01	25	P350	0 0 0 0 0	
6.133E-03	1.338E+00	37	J030	1 2 2 2 2	intrinsic

2390. C₁₁H₁₀N₂S

1-Naphthylthiourea

ANTU

RN: 86-88-4 MP (°C): 198

MW: 202.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.966E-03	6.000E-01	rt	M161	0 0 0 0 2	

2391. C₁₁H₁₀N₄O₄S

2-Sulfanilamido-5-nitropyridine

Benzenesulfonamide, 4-amino-*N*-(5-nitro-2-pyridinyl)-

RN: 39588-36-8 MP (°C):

MW: 294.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.257E-04	3.700E-02	37	R058	1 2 1 1 1	

2392. C₁₁H₁₁ClO₃

Alclofenac

(4-Allyloxy-3-chlorophenyl)acetic acid

(3-Chloro-4-allyloxyphenyl)acetic acid

RN: 22131-79-9 **MP (°C):****MW:** 226.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.850E-05	1.099E-02	5	F306	1 0 1 2 2	
5.780E-05	1.310E-02	25	C314	0 0 0 0 0	
5.780E-05	1.310E-02	25	C314	0 0 0 0 0	
6.200E-05	1.405E-02	25	F306	1 0 1 2 2	intrinsic
8.000E-05	1.813E-02	37	F306	1 0 1 2 2	intrinsic

2393. C₁₁H₁₁N

2,4-Dimethylquinoline

Quinoline, 2,4-dimethyl-

RN: 1198-37-4 **MP (°C):** 264**MW:** 157.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-02	1.795E+00	25	K119	1 0 0 0 2	

2394. C₁₁H₁₁N

2,7-Dimethylquinoline

Quinoline, 2,7-dimethyl-

RN: 93-37-8 **MP (°C):** 58**MW:** 157.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-02	1.795E+00	25	P051	2 1 1 2 2	
1.142E-02	1.795E+00	25.00	P007	2 1 2 2 2	

2395. C₁₁H₁₁NO

Aziridine, 1-(1-oxo-3-phenyl-2-propenyl)-

N-Cyclopropylcinnamamide

RN: 53162-40-6 **MP (°C):****MW:** 173.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.150E-03	5.456E-01	ns	H350	0 0 0 0 0	

2396. C₁₁H₁₁NO₂

Phensuximide

Milontin

N-Methyl-2-phenyl-succinimide

RN: 86-34-0 MP (°C): 71–73

MW: 189.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-02	4.200E+00	25	P061	0 0 0 0 0	

2397. C₁₁H₁₁NO₂SButyric acid, *p*-isothiocyanatophenyl ester

RN: 96933-13-0 MP (°C):

MW: 221.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.814E-02	25	K032	2 2 0 1 1	

2398. C₁₁H₁₁NO₄Acetamide, *N*-acetyl-2-(benzoyloxy)-

RN: 68659-48-3 MP (°C): 104.5

MW: 221.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.978E-03	8.800E-01	22	N317	1 1 2 1 2	

2399. C₁₁H₁₁NO₄S

4-Thiazolidinecarboxylic acid, 2-(4-carboxyphenyl)-

Thiazolidine-4-carboxylic acid, 2-(4-carboxyphenyl)-

RN: 118845-10-6 MP (°C):

MW: 253.28 BP (°C): 551.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	1.520E-01	21	B414	1 0 0 1 1	fast decomposition, results from gravimetric determination

2400. C₁₁H₁₁NO₅

Benzoxydiglycine

RN:

MP (°C):

MW: 237.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.391E-02	3.300E+00	25.1	N026	0 0 0 0 0	

2401. C₁₁H₁₁NO₅

Benzoic acid, 2-(acetyloxy)-, 2-amino-2-oxoethyl ester

(O-Acetyl salicyloyloxy)acetamide

RN: 50785-22-3 MP (°C): 128.5

MW: 237.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.619E-02	3.840E+00	21	N335	0 0 0 0 0	

2402. C₁₁H₁₁N₃OS

Seedvax

2-Amino-4-methyl-5-carboxanilidothiazole

RN: 21452-14-2 MP (°C): 221

MW: 233.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.282E-03	9.990E-01	ns	M061	0 0 0 0 0	

2403. C₁₁H₁₁N₃O₂S

Sulfapyridine

2-(Aminobenzene-4'-sulfamido)-pyridine

2-[Aminobenzol-4'-sulfamid]-pyridin

Sulphapyridine

2-Sulfapyridine

N-(2-Pyridyl)sulfanilamide

RN: 144-83-2 MP (°C): 192

MW: 249.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.819E-04	1.700E-01	16	H114	1 0 0 0 2	
2.006E-03	5.000E-01	20	C103	1 2 0 0 2	
1.323E-03	3.299E-01	20	D041	1 0 0 0 1	
8.023E-04	2.000E-01	20	F073	1 2 2 2 2	
1.075E-03	2.680E-01	25	C102	2 0 2 2 2	
1.049E-03	2.615E-01	25	M440	0 0 0 0 0	
1.645E-03	4.100E-01	35	H114	1 0 0 0 1	

(continued)

2403. C₁₁H₁₁N₃O₂S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-03	4.860E-01	37	C102	2 0 2 2 2	
1.805E-03	4.500E-01	37	D084	1 0 1 0 1	
1.985E-03	4.948E-01	37	F072	1 0 0 0 2	
1.985E-03	4.948E-01	37	F075	1 0 2 2 2	
2.006E-03	5.000E-01	37	F300	1 0 0 0 0	
4.047E-03	1.009E+00	37	G037	2 2 2 1 0	EFG, form V
6.128E-03	1.528E+00	37	G073	2 2 2 1 0	EFG, amorphous
3.807E-03	9.491E-01	37	G073	2 2 2 1 0	EFG, form II
3.807E-03	9.491E-01	37	G073	2 2 2 1 0	EFG, form I
2.090E-03	5.210E-01	37	K095	2 0 0 0 2	intrinsic
2.447E-03	6.100E-01	37	M057	1 0 0 0 2	pH 5.5
2.607E-03	6.500E-01	37	R044	0 0 0 0 0	
6.417E-04	1.600E-01	37.50	M142	1 0 0 0 1	
2.165E-03	5.397E-01	37.50	M142	1 0 0 0 1	
2.006E-03	5.000E-01	38	K006	1 0 0 0 2	
4.412E-03	1.100E+00	40	C103	1 2 0 0 2	
4.212E-02	1.050E+01	100	C103	1 2 0 0 2	
3.972E-02	9.901E+00	100	D041	1 0 0 0 0	
1.995E-03	4.974E-01	ns	R427	0 0 0 0 0	
1.484E-03	3.699E-01	rt	N015	0 0 2 2 2	

2404. C₁₁H₁₁N₃O₃S₂

Acetyl sulfathiazole

Sulfathiazol acetyle

N4-Acetyl sulfathiazole

N4-Acetyl sulphathiazole

RN: 127-76-4

MP (°C):

MW: 297.36

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.363E-04	1.000E-01	37	D084	1 0 1 0 1	
2.186E-04	6.500E-02	37	F075	1 0 2 2 1	
2.354E-04	7.000E-02	37	L091	1 0 0 0 0	pH 5.5
1.951E-04	5.800E-02	37	M057	1 0 0 0 1	pH 5.5
2.018E-04	6.000E-02	37.50	M142	1 0 0 0 0	
2.388E-04	7.100E-02	38	K006	1 0 0 0 1	

2405. C₁₁H₁₁N₃O₃S

5-Sulfanilamido-2-hydroxypyridine

RN: 71119-20-5 MP (°C):

MW: 265.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.725E-03	2.580E+00	37	R058	1 2 1 1 1	

2406. C₁₁H₁₁N₅

Phenazopyridine

3-(Phenylazo)-2,6-pyridinediamine

RN: 94-78-0 MP (°C): 235

MW: 213.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.240E+00	9.042E+02	25	B443	0 0 0 0 0	
1.738E-04	3.706E-02	ns	R427	0 0 0 0 0	

2407. C₁₁H₁₂ClNO₄

Chloroethyl acetaminophen

Carbonic acid, 4-(acetylamino)phenyl 2-chloroethyl ester

Acetanilide, 4'-hydroxy-, 2-chloroethyl carbonate (ester)

RN: 17243-29-7 MP (°C): 122.5–123

MW: 257.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.514E-03	3.900E-01	37	D029	0 0 0 0 0	

2408. C₁₁H₁₂Cl₂N₂O₅

Chloramphenicol

D-(-)-Threo-1-(*p*-nitrophenyl)-2-dichloroacetamido-1,3-propanediol

Amphicol

Leukomycin

Cloramical

Intramycin

RN: 56-75-7 MP (°C): 150.5

MW: 323.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.717E-03	2.494E+00	20	D041	1 0 0 0 1	
5.570E-03	1.800E+00	23	M168	2 0 0 0 0	EFG
1.200E-02	3.878E+00	25	A352	0 0 0 0 0	
7.717E-03	2.494E+00	25	I312	0 0 0 0 0	
1.156E-02	3.736E+00	25.5	J011	1 0 2 1 2	pH 4.7
1.370E-02	4.427E+00	30	K020	1 0 1 1 0	EFG
1.238E-02	4.000E+00	37	G010	1 0 1 1 0	EFG
7.737E-03	2.500E+00	ns	K444	0 0 0 0 0	

2409. C₁₁H₁₂Cl₂O₃

2,4-d Isopropyl ester

2,4-d-Isopropyl ester

2,4-Dichlorophenoxyacetic acid isopropyl ester

2,4-Dichlorophenoxyacetic acid *iso*-propyl ester

RN: 94-11-1 MP (°C):

MW: 263.12 BP (°C): 139

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	2.736E-02	ns	M120	0 0 1 1 2	
1.419E-04	3.734E-02	ns	M120	0 0 1 1 2	

2410. C₁₁H₁₂I₃NO₂

Ipanoic acid

β-(3-Amino-2,4,6-triiodophenyl)-α-ethylpropionic acid

Bilijodon

Cholevid

Choladine

Colepax

RN: 96-83-3 MP (°C): 155.2

MW: 570.94 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-04	3.483E-01	37	J016	1 0 0 0 1	pH 7.4
2.627E-05	1.500E-02	ns	H055	0 0 0 0 0	

2411. C₁₁H₁₂NO₄PS₂

Phosmet

Phosphorodithioic acid *S*-[(1,3-dihydro-1,3-dioxo-2*H*-isoindol-2-yl)methyl] *O,O*-dimethyl ester

Decemthion

Smidan

Appa

Imidan

RN: 732-11-6 MP (°C):

MW: 317.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.690E-05	2.440E-02	20	B300	2 1 1 1 2	
7.878E-05	2.500E-02	25	M061	1 0 0 0 1	
7.878E-05	2.500E-02	25	M161	1 0 0 0 1	
7.878E-05	2.500E-02	ns	F071	0 1 2 1 1	
7.943E-05	2.521E-02	ns	R427	0 0 0 0 0	

2412. C₁₁H₁₂N₂O

Antipyrine

Antipyrin

2,3-Dimethyl-1-phenyl-3-pyrazolin-5-one

1,2-Dihydro-1,5-dimethyl-2-phenyl-3H-pyrazol-3-one

Phenazone

RN: 60-80-0**MP (°C):** 114**MW:** 188.23**BP (°C):** 319

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E+00	2.918E+02	2.5	K075	1 0 0 0 2	
1.968E+00	3.705E+02	4.62	M109	2 1 1 1 0	EFG
1.472E-01	2.771E+01	5	L089	1 0 0 0 2	<i>sic</i>
1.613E+00	3.036E+02	6.1	K075	1 0 0 0 2	
1.777E-01	3.344E+01	10	L089	1 0 0 0 2	<i>sic</i>
2.084E+00	3.922E+02	11.74	M109	2 1 1 1 0	EFG
2.261E+00	4.256E+02	14.20	M109	2 1 1 1 0	EFG
1.771E+00	3.333E+02	20	D041	1 0 0 0 0	
2.205E-01	4.150E+01	20	L089	1 0 0 0 2	<i>sic</i>
2.472E+00	4.654E+02	20.96	M109	2 1 1 1 0	EFG
2.621E-01	4.934E+01	25	L089	1 0 0 0 2	<i>sic</i>
3.294E+00	6.200E+02	25	P012	0 0 0 0 0	
3.294E+00	6.200E+02	25	P016	1 0 0 1 2	
3.559E+00	6.700E+02	25	P020	2 0 1 1 2	
2.717E+00	5.114E+02	25.35	M109	2 1 1 1 0	EFG
3.020E+00	5.685E+02	29.87	M109	2 1 1 1 0	EFG
2.621E-01	4.934E+01	30	L089	1 0 0 0 2	<i>sic</i>
2.983E-01	5.616E+01	35	L089	1 0 0 0 2	<i>sic</i>
3.968E+00	7.468E+02	39.34	M109	2 1 1 1 0	EFG
3.359E-01	6.323E+01	40	L089	1 0 0 0 2	<i>sic</i>
5.637E-01	1.061E+02	50	L089	1 0 0 0 2	<i>sic</i>
1.493E+00	2.811E+02	.0	K075	1 0 0 0 2	
2.656E+00	5.000E+02	rt	D021	0 0 1 1 2	

2413. C₁₁H₁₂N₂O₂

DL-Tryptophan

1H-Indole-3-alanine

DL- α -Amino-3-indolepropionic acid**RN:** 54-12-6**MP (°C):** 289**MW:** 204.23**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-02	2.083E+00	20	N006	0 0 0 0 0	
1.140E-02	2.328E+00	25	N006	0 0 0 0 0	
1.221E-02	2.494E+00	30	D041	1 0 0 0 1	
1.250E-02	2.553E+00	30	N006	0 0 0 0 0	
1.200E-02	2.451E+00	30	N009	0 0 0 0 0	
1.640E-02	3.349E+00	40	N006	0 0 0 0 0	
1.570E-02	3.206E+00	40	N009	0 0 0 0 0	
2.150E-02	4.391E+00	50	N006	0 0 0 0 0	

2414. C₁₁H₁₂N₂O₂

Tryptophan

2-Amino-3-(1H-indol-3-yl)-propanoic acid

3-Indol-3-ylalanine

L-β-3-indolylalanine

Trp

(S)-(-)-Tryptophan

RN: 73-22-3**MP (°C):****MW:** 204.23**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.015E-02	8.200E+00	0	F300	1 0 0 0 1	
6.042E-02	1.234E+01	20	B032	1 2 2 1 2	
6.395E-02	1.306E+01	22.5	P045	0 0 2 1 2	
6.551E-02	1.338E+01	25	B032	1 2 2 1 2	
5.519E-02	1.127E+01	25	D041	1 0 0 0 2	
5.337E-02	1.090E+01	25	F300	1 0 0 0 2	
6.665E-02	1.361E+01	25	G092	2 1 1 1 1	
6.665E-02	1.361E+01	25	G315	0 0 0 0 0	
5.519E-02	1.127E+01	25	H070	1 0 0 0 2	
6.267E-02	1.280E+01	25.1	N024	0 0 0 0 0	
6.757E-02	1.380E+01	25.1	N025	0 0 0 0 0	
6.757E-02	1.380E+01	25.1	N026	0 0 0 0 0	
6.665E-02	1.361E+01	25.1	N027	1 1 2 2 2	
1.787E-01	3.650E+01	27	D036	0 0 0 0 0	
5.386E-02	1.100E+01	28	L081	2 1 2 2 2	
7.056E-02	1.441E+01	29.80	B032	1 2 2 1 2	
8.100E-02	1.654E+01	30	N009	0 0 0 0 0	
9.480E-02	1.936E+01	40	N009	0 0 0 0 0	
8.226E-02	1.680E+01	50	F300	1 0 0 0 2	
1.122E-01	2.291E+01	50	N009	0 0 0 0 0	
1.200E-01	2.450E+01	70	F300	1 0 0 0 2	
1.334E-01	2.724E+01	75	D041	1 0 0 0 2	
2.448E-01	5.000E+01	100	F300	1 0 0 0 1	

2415. C₁₁H₁₂N₂O₂

5-Ethyl-5-phenylhydantoin

2,4-Imidazolidinedione, 5-ethyl-5-phenyl-

Nirvanol

5-Phenyl-5-ethylhydantoin

Normephentyoin

RN: 631-07-2**MP (°C):****MW:** 204.23**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.938E-03	8.044E-01	37	F183	1 0 1 1 1	intrinsic

2416. C₁₁H₁₂N₂O₄Acetamide, *N*-(2-amino-2-oxoethyl)-2-(benzoyloxy)-**RN:** 106231-53-2 **MP (°C):** 151.5**MW:** 236.23 **BP (°C):** 568.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.175E-02	7.500E+00	22	B427	1 0 0 1 1	
3.175E-02	7.500E+00	22	N317	1 1 2 1 2	in 0.01M HCl

2417. C₁₁H₁₂N₄O₂S

2-Sulfanilamido-5-aminopyridine

Benzenesulfonamide, 4-amino-*N*-(5-amino-2-pyridinyl)-**RN:** 16840-28-1 **MP (°C):****MW:** 264.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.581E-02	4.180E+00	37	R058	1 2 1 1 2	

2418. C₁₁H₁₂N₄O₂S

4-Sulfanilamido-2-methylpyrimidine

Benzenesulfonamide, 4-amino-*N*-(2-methyl-4-pyrimidinyl)-**RN:** 599-84-8 **MP (°C):****MW:** 264.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.357E-02	6.230E+00	37	R046	1 2 1 1 2	

2419. C₁₁H₁₂N₄O₂S

Sulfamethylpyrimidine

Ulfamerazine

Sulfamerazine

RN: 127-79-7 **MP (°C):** 234**MW:** 264.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.967E-04	2.370E-01	20	F073	1 2 2 2 2	
7.641E-04	2.020E-01	20	L058	1 0 1 1 2	
8.012E-04	2.118E-01	25	M440	0 0 0 0 0	
1.400E-03	3.700E-01	37	L091	1 0 0 0 1	pH 5.5
1.203E-03	3.180E-01	37	R045	1 2 1 1 2	
1.381E-03	3.650E-01	37	S192	1 0 1 1 2	pH 6.0
1.551E-03	4.100E-01	38	K006	1 0 0 0 1	

2420. C₁₁H₁₂N₄O₃S₂

N4-Acetyl sulfamethizole

Acetyl sulfamethylthiazole

RN: 39719-87-4 **MP (°C):**
MW: 312.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.313E-03	4.100E-01	37	B046	1 0 2 2 1	pH 4.5

2421. C₁₁H₁₂N₄O₃S

Sulfamethoxypyridazine

Sulphamethoxypyridazine

4-Amino-N-(6-methoxy-3-pyridazinyl)-benzenesulfonamide

RN: 80-35-3 **MP (°C):** 182.5
MW: 280.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.067E-03	5.795E-01	25	E314	0 0 0 0 0	intrinsic
2.569E-02	7.200E+00	37	B046	1 0 2 2 2	pH 4.5

2422. C₁₁H₁₂N₄O₃S

Sulfamer

Sulphamethoxydiazine

RN: 651-06-9 **MP (°C):** 213
MW: 280.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.677E-03	4.700E-01	30	M113	2 2 2 2 0	form III, EFG, 0.1N HCl
2.604E-03	7.300E-01	30	M113	2 2 2 2 0	form II, EFG, 0.1N HCl
1.891E-03	5.300E-01	30	M113	2 2 2 2 0	form I, EFG, 0.1N HCl
2.462E-03	6.900E-01	30	M113	2 2 2 2 0	EFG, 0.1N HCl, amorphous
3.211E-04	9.000E-02	37.5	C081	1 0 1 0 0	EFG, form III
6.243E-04	1.750E-01	37.5	C081	1 0 1 0 0	EFG, form II
4.281E-04	1.200E-01	37.5	C081	1 0 1 0 0	EFG, form I

2423. C₁₁H₁₂N₄O₃S

5-Sulfanilamido-2-methoxypyrimidine

Benzenesulfonamide, 4-amino-N-(2-methoxy-5-pyrimidinyl)-

RN: 71119-37-4 **MP (°C):**
MW: 280.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.282E-04	9.200E-02	37	R046	1 2 1 1 1	

2424. C₁₁H₁₂N₄O₃S

2-Sulfanilamido-4-methoxypyrimidine

Benzenesulfonamide, 4-amino-N-(4-methoxy-2-pyrimidinyl)-

RN: 3213-22-7 MP (°C):

MW: 280.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.493E-04	1.820E-01	37	R046	1 2 1 1 2	

2425. C₁₁H₁₂N₄O₅

2,5-Diacetoxymethyl allopurinol

4H-Pyrazolo[3,4-d]pyrimidin-4-one, 2,5-bis[(acetoxy)methyl]-2,5-dihydro-

RN: 98827-24-8 MP (°C): 153–154

MW: 280.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E-02	2.900E+00	22	B322	0 0 0 0 0	

2426. C₁₁H₁₂N₆O₂S

6-Sulfapurine

RN: MP (°C):

MW: 292.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.447E-05	1.300E-02	20	F073	1 2 2 2 1	

2427. C₁₁H₁₂O₂

Cinnamyl acetate

3-Phenylallyl acetate

3-Phenyl-2-propenyl acetate

1-Acetoxy-3-phenyl-2-propene

3-Phenyl-2-propen-1-ol acetate

NSC 46109

RN: 103-54-8 MP (°C):

MW: 176.22 BP (°C): 170 (°50 torr)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.762E-01	25	D407	1 0 2 2 2	
1.000E-03	1.762E-01	ns	S460	0 0 0 0 0	

2428. C₁₁H₁₂O₂

Ethyl cinnamate

Ethyl (E)-cinnamate

Ethyl 3-phenyl propenoate

Ethyl phenylacrylate

RN: 103-36-6 **MP (°C):** 6
MW: 176.22 **BP (°C):** 271

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-03	1.780E-01	25	A002	1 2 1 1 2	

2429. C₁₁H₁₂O₄

3,5-Dimethoxycinnamic acid

Predominantly *trans* isomer

RN: 16909-11-8 **MP (°C):** 174.5
MW: 208.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.510E-04	3.144E-02	25	R070	0 0 0 0 0	

2430. C₁₁H₁₂O₄

Ethyl acetylsalicylate

Acetyl salicylic acid, ethyl ester

RN: 529-68-0 **MP (°C):**
MW: 208.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.594E-02	3.320E+00	37	G430	0 0 0 0 0	pH 4.5

2431. C₁₁H₁₂O₄Propionyl-*r*-mandelic acid

RN: **MP (°C):** 126
MW: 208.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-02	2.892E+00	0	A043	1 2 1 1 1	
1.389E-02	2.892E+00	0	L035	1 2 2 1 1	
1.675E-02	3.488E+00	10	A043	1 2 1 1 1	
1.675E-02	3.488E+00	10	L035	1 2 2 1 1	
1.770E-02	3.686E+00	15	A043	1 2 1 1 1	
1.770E-02	3.686E+00	15	L035	1 2 2 1 1	
1.818E-02	3.786E+00	20	A043	1 2 1 1 1	
1.818E-02	3.786E+00	20	L035	1 2 2 1 1	
2.484E-02	5.173E+00	25	A043	1 2 1 1 1	

(continued)

2431. C₁₁H₁₂O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.484E-02	5.173E+00	25	L035	1 2 2 1 1	
2.817E-02	5.865E+00	30	A043	1 2 1 1 1	
2.817E-02	5.865E+00	30	L035	1 2 2 1 1	
3.528E-02	7.346E+00	35	A043	1 2 1 1 1	
3.528E-02	7.346E+00	35	L035	1 2 2 1 1	
5.789E-02	1.205E+01	40	A043	1 2 1 1 2	
5.789E-02	1.205E+01	40	L035	1 2 2 1 2	
8.724E-02	1.816E+01	45	A043	1 2 1 1 2	
8.724E-02	1.816E+01	45	L035	1 2 2 1 2	
1.606E-01	3.344E+01	50	A043	1 2 1 1 2	
1.606E-01	3.344E+01	50	L035	1 2 2 1 2	

2432. C₁₁H₁₂O₄S

Benzoic acid, 2-(acetyloxy)-, (methylthio)methyl ester

RN: 76432-30-9 MP (°C):

MW: 240.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.289E-03	5.500E-01	21	N335	0 0 0 0 0	

2433. C₁₁H₁₂O₅S

2-(Acetoxy)-benzoic acid, (methylsulfinyl)methyl ester

RN: 76432-33-2 MP (°C): 80.5

MW: 256.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.651E-02	4.230E+00	21	N335	0 0 0 0 0	

2434. C₁₁H₁₂O₆S

2-(Acetoxy)-benzoic acid, (methylsulfonyl)methyl ester

RN: 76432-35-4 MP (°C): 150

MW: 272.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.040E-04	1.100E-01	21	N335	0 0 0 0 0	

2435. C₁₁H₁₃ClO₃

Bexone

4-(2-Methyl-4-chlorophenoxy)butyric acid

4-(MCPB)

MCPB

RN: 94-81-5**MP (°C):****MW:** 228.68**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.099E-04	4.800E-02	25	B164	1 0 1 1 1	
1.924E-04	4.400E-02	ns	L024	0 0 0 0 1	
1.924E-04	4.400E-02	ns	M061	0 0 0 0 1	
1.924E-04	4.400E-02	rt	M161	0 0 0 0 1	

2436. C₁₁H₁₃FN₂O₄

1-Cyclohexyloxycarbonyl-5-fluorouracil

1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, cyclohexyl ester

RN: 109232-74-8 **MP (°C):****MW:** 256.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.590E-03	9.200E-01	22	B332	1 1 0 0 1	pH 4.0

2437. C₁₁H₁₃F₃N₂O₃S

Mefluidide

N-(2,4-Dimethyl-5-(((trifluoromethyl)sulfonyl)amino)phenyl)acetamide

Vistar

Embark

MBR 12325

Methafluoridamid

RN: 53780-34-0 **MP (°C):** 184**MW:** 310.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.801E-04	1.800E-01	23	M161	1 0 0 0 2	

2438. C₁₁H₁₃F₃N₄O₄

Dinitramine

1,3-Benzenediamine, *N*1,*N*1-diethyl-2,6-dinitro-4-(trifluoromethyl)-*N*3,*N*3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-*m*-phenylenediamine*N*3,*N*3-Diethyl-2,4-dinitro-6-(trifluoromethyl)-1,3-phenylenediamine

USB 3584

RN: 29091-05-2 **MP (°C):** 98.5**MW:** 322.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.414E-06	1.100E-03	25	M161	1 0 0 0 1	

2439. C₁₁H₁₃NO*N,N*-Dimethylcinnamide

Cinnamic acid dimethylamide

N,N-Dimethyl-3-phenyl-2-propenamide**RN:** 13156-74-6 **MP (°C):****MW:** 175.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.670E-02	2.926E+00	ns	H350	0 0 0 0 0	

2440. C₁₁H₁₃NO*N*-Ethylcinnamamide

N-Ethyl-3-phenyl-2-propenamide

RN: 23784-45-4 **MP (°C):****MW:** 175.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.390E-03	1.120E+00	ns	H350	0 0 0 0 0	

2441. C₁₁H₁₃NO₂S2-*p*-Tolyl-4-thiazolidinecarboxylic acid

4-Thiazolidinecarboxylic acid, 2-(4-methylphenyl)-

RN: 67189-37-1 **MP (°C):****MW:** 223.30 **BP (°C):** 444.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	4.019E-01	21	B414	1 0 0 1 1	very fast and extent decomposition, uncertain value

2442. C₁₁H₁₃NO₃

Acetaminophen propionate

Propionic acid, *p*-acetamidophenyl ester**RN:** 54942-42-6 **MP (°C):** 130**MW:** 207.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.544E-03	3.200E-01	25	B010	1 1 1 1 0	

2443. C₁₁H₁₃NO₃

Acetamide, 2-(benzoyloxy)-*N*-ethyl-
2-(Benzoyloxy)-*N*,*N*-dimethylacetamide

RN: 64649-57-6 **MP (°C):** 106
MW: 207.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.791E-03	1.200E+00	22	B427	1 0 0 1 1	in 0.01M HCl
5.791E-03	1.200E+00	22	N317	1 1 2 1 2	

2444. C₁₁H₁₃NO₃

Acetamide, 2-(benzoyloxy)-*N,N*-dimethyl-
2-(Benzoyloxy)-*N,N*-dimethylacetamide

RN: 106231-54-3 **MP (°C):** 81.5
MW: 207.23 **BP (°C):** 351.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.246E-02	8.800E+00	22	B427	1 0 0 1 1	in 0.01M HCl
4.246E-02	8.800E+00	22	N317	1 1 2 1 2	

2445. C₁₁H₁₃NO₃S

4-Thiazolidinecarboxylic acid, 2-(4-methoxyphenyl)-
Thiazolidine-4-carboxylic acid, 2-(4-methoxyphenyl)-

RN: 65884-40-4 **MP (°C):** 165–166
MW: 239.30 **BP (°C):** 466.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	9.572E-02	21	B414	1 0 0 1 1	fast decomposition

2446. C₁₁H₁₃NO₄

Bendiocarb

2,2-Dimethyl-1,3-benzodioxol-4-ol methylcarbamate

Fuam

Multimet

Garvox

RN: 22781-23-3 **MP (°C):** 129.5
MW: 223.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.792E-04	4.000E-02	25	M161	1 0 0 0 1	
1.792E-04	4.000E-02	25	W310	1 0 0 0 0	

2447. C₁₁H₁₃NO₄

N,N-Dimethyl glycolamide salicylate

2-Hydroxybenzoic acid, 2-(dimethylamino)-2-oxoethyl ester

RN: 114665-08-6 MP (°C): 68

MW: 223.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.971E-02	4.400E+00	21	B331	1 2 2 1 0	pH 7.4
1.971E-02	4.400E+00	21	B331	0 0 0 0 0	

2448. C₁₁H₁₃NO₄

Ethyl acetaminophen

Carbonic acid, 4-(acetylamino)phenyl ethyl ester

Acetanilide, 4'-hydroxy-, ethyl carbonate (ester)

RN: 17243-26-4 MP (°C): 121–122

MW: 223.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.928E-03	1.100E+00	37	D029	0 0 0 0 0	

2449. C₁₁H₁₃NO₄

Dioxacarb

2-(1,3-Dioxolan-2-yl)phenyl methylcarbamate

2-(1,3-Dioxolan-2-yl)-phenyl N-methylcarbamate

Elocron

Famid

RN: 6988-21-2 MP (°C): 114.5

MW: 223.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.688E-02	6.000E+00	20	M161	1 0 0 0 0	

2450. C₁₁H₁₃NO₄S

4-Thiazolidinecarboxylic acid, 2-(2-hydroxy-3-methoxyphenyl)-

Thiazolidine-4-carboxylic acid, 2-(2-hydroxy-3-methoxyphenyl)-

RN: 72678-93-4 MP (°C):

MW: 255.29 BP (°C): 435.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	1.532E+00	2.1	B414	1 0 0 1 1	fast decomposition

2451. C₁₁H₁₃N₃O

Ampyrone

4-Aminoantipyrine

Aminophenazone

RN: 83-07-8**MP (°C):** 109**MW:** 203.25**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.053E-01	1.840E+02	5.39	M109	2 1 1 1 0	EFG
1.088E+00	2.211E+02	10.93	M109	2 1 1 1 0	EFG
1.252E+00	2.544E+02	14.20	M109	2 1 1 1 0	EFG
1.527E+00	3.103E+02	20.96	M109	2 1 1 1 0	EFG
2.076E+00	4.218E+02	25.35	M109	2 1 1 1 0	EFG
2.384E+00	4.845E+02	29.87	M109	2 1 1 1 0	EFG
2.400E-01	4.878E+01	30	I010	2 1 2 2 1	EFG, <i>sic</i>
2.862E+00	5.816E+02	39.34	M109	2 1 1 1 0	EFG

2452. C₁₁H₁₃N₃O₃S

Sulfamoxole

Sulfuno

N-(4,5-Dimethyloxazol-2-yl)sulfanilamide

RN: 729-99-7 **MP (°C):** 193**MW:** 267.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.595E-03	9.610E-01	20	K028	2 1 2 1 2	pH 6.0, form I
3.430E-03	9.170E-01	20	K028	2 1 2 1 2	pH 3.8, form I
3.277E-03	8.760E-01	20	K028	2 1 2 1 2	pH 6.0, form II
3.165E-03	8.460E-01	20	K028	2 1 2 1 2	pH 3.8, form II
6.274E-03	1.677E+00	20	K028	2 1 2 1 2	pH 7.3, form I
5.447E-03	1.456E+00	20	K028	2 1 2 1 2	pH 7.3, form II
3.427E-03	9.162E-01	20	M042	1 0 0 0 2	pH 3.8, form I, mp 205-211 C
3.162E-03	8.453E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 188-195 C

2453. C₁₁H₁₃N₃O₃S

Sulfisoxazole

4-Amino-N-(3,4-dimethyl-5-isoxazolyl)benzenesulfonamide

3,4-Dimethyl-5-sulfanilamidoisoxazole

Gantrisin

Urogan

Urisoxin

RN: 127-69-5 **MP (°C):** 194**MW:** 267.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.235E-03	3.300E-01	37	B046	1 0 2 2 1	pH 4.5
3.142E-04	8.400E-02	37	K022	1 0 1 1 0	intrinsic
1.092E-03	2.920E-01	37	K091	1 0 0 0 2	

2454. C₁₁H₁₃N₃O₃S

N1-Methyl-N1-(5-methyl-3-isoxazolyl)sulfanilamide

N1-Methylsulfamethoxazole

RN: 51543-31-8 MP (°C):

MW: 267.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.280E-04	1.679E-01	37	K095	2 0 0 0 2	intrinsic

2455. C₁₁H₁₃N₅O₂

Carbovir

9-[4α-(Hydroxymethyl)-cyclopent-2-ene-1α-yl]guanine

RN: 118353-05-2 MP (°C):

MW: 247.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.015E-03	1.240E+00	25	A338	0 0 0 0 0	

2456. C₁₁H₁₃N₅O₅

Arabinosyladenine 5'-formate

Arabinosyladenine 5'-O-formate ester

NSC 171240

RN: 55648-40-3 MP (°C): 168–170

MW: 295.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.152E-01	3.400E+01	ns	R030	0 0 0 0 0	

2457. C₁₁H₁₄ClNO

Propachlor

2-Chloro-*N*-isopropylacetanilide*N*-Isopropyl-2-chloroacetanilide*N*-Isopropyl-α-chloroacetanilide

RN: 1918-16-7 MP (°C): 67

MW: 211.69 BP (°C): 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-03	7.000E-01	20	B200	1 0 0 0 2	
3.307E-03	7.000E-01	20	M161	1 0 0 0 2	
3.304E-03	6.995E-01	ns	J008	0 0 0 0 0	
3.304E-03	6.995E-01	ns	M061	0 0 0 0 0	
2.362E-03	5.000E-01	ns	M110	0 0 0 0 0	EFG

2458. C₁₁H₁₄N₂O

Cytisine

Cytisin

RN: 485-35-8

MP (°C): 155

MW: 190.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.308E+00	4.390E+02	16	F300	1 0 0 0 2	

2459. C₁₁H₁₄N₂O₃S

Sulfadicramide

2-Butenamide, *N*-[(4-aminophenyl)sulfonyl]-3-methyl-

N-Sulfanilyl-β,β-dimethylacrylamide

Sulfirgamid

Irgamide

Sulfirgamide

RN:	115-68-4	MP (°C):	184.5
MW:	254.31	BP (°C):	

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-03	2.610E-01	20	F073	1 2 2 2 2	

2460. C₁₁H₁₄N₄O₂S₂4-Amino-*N*-(5-isopropyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide

N1-(5-Isopropyl-1,3,4-thiadiazol-2-yl)sulfanilamide

Sulfaisopropylthiadiazole

Glyprothiazole

PASIT

RP 2254

RN:	80-34-2	MP (°C):	
MW:	298.39	BP (°C):	

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.330E-04	2.187E-01	37	A046	2 0 1 1 2	

2461. C₁₁H₁₄N₄O₂S₂4-Amino-*N*-(5-propyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide

N1-(5-Propyl-1,3,4-thiadiazol-2-yl)sulfanilamide

RN:	71119-32-9	MP (°C):	
MW:	298.39	BP (°C):	

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.980E-04	2.680E-01	37	A046	2 0 1 1 2	

2462. C₁₁H₁₄N₄O₃

2-Pivaloyloxymethyl allopurinol

Propanoic acid, 2,2-dimethyl-, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-2-yl)methyl ester

RN: 98827-15-7 MP (°C): 180–181

MW: 250.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.793E-03	1.700E+00	22	B322	0 0 0 0 0	

2463. C₁₁H₁₄N₄O₃

1-Pivaloyloxymethyl allopurinol

Propanoic acid, 2,2-dimethyl-, (4,5-dihydro-4-oxo-2H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester

RN: 98827-18-0 MP (°C): 185–187

MW: 250.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.078E-03	5.200E-01	22	B322	0 0 0 0 0	

2464. C₁₁H₁₄N₄O₅

6-Methoxypurine arabinoside

9H-Purine, 9-β-D-arabinofuranosyl-6-methoxy-

RN: 91969-06-1 MP (°C):

MW: 282.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.980E-02	1.406E+01	37	C348	0 0 0 0 0	pH 7.00

2465. C₁₁H₁₄O

o-2-Pentenylphenol

Phenol, 2-(2-pentenyl)-

RN: 62536-86-1 MP (°C):

MW: 162.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.054E-03	3.332E-01	25	L021	1 0 0 0 0	

2466. C₁₁H₁₄O₂

δ-Phenylvaleric acid

Benzenepentanoic acid

5-Phenylvaleric acid

RN: 2270-20-4 MP (°C): 59

MW: 178.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.969E-03	1.777E+00	30	D033	2 2 1 2 2	
1.159E-02	2.066E+00	40	D033	2 2 1 2 2	

2467. C₁₁H₁₄O₂

4-Butylbenzoic acid

RN: 20651-71-2 MP (°C): 100

MW: 178.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-04	1.482E-01	ns	R427	0 0 0 0 0	

2468. C₁₁H₁₄O₂

Ethyl hydrocinnamate

Ethyl 3-phenylpropionate

Benzenepropanoic acid, ethyl ester

RN: 2021-28-5 MP (°C):

MW: 178.23 BP (°C): 122

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.234E-03	2.200E-01	25	A002	1 2 1 1 1	

2469. C₁₁H₁₄O₃*n*-Butyl salicylate

2-Hydroxy-benzoic acid, butyl ester

Salicylic acid *n*-butyl ester

Butyl salicylate

Benzoic acid, 2-hydroxy-, butyl ester

RN: 2052-14-4 MP (°C):

MW: 194.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.442E-02	2.800E+00	37	D009	1 2 1 1 1	0.1N HCl

2470. C₁₁H₁₄O₃

2-Hydroxy-3-isopropyl-6-methylbenzoic acid

o-Thymotinic acid

RN: 548-51-6 **MP (°C):**
MW: 194.23 **BP (°C):** 316.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.57E-03	>5.00E-01	ns	B404	0 2 1 1 0	

2471. C₁₁H₁₄O₃

Butylparaben

Bu-paraben

Butyl 4-hydroxybenzoate

RN: 94-26-8 **MP (°C):** 68.5
MW: 194.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.040E-04	1.367E-01	15	B355	0 0 0 0 0	
8.350E-04	1.622E-01	20	B355	0 0 0 0 0	
1.065E-03	2.069E-01	20	C006	1 2 1 1 2	
1.277E-03	2.481E-01	25	A059	1 0 1 1 1	
1.050E-03	2.039E-01	25	B355	0 0 0 0 0	
8.751E-04	1.700E-01	25	D081	1 2 2 1 2	
1.130E-03	2.195E-01	25	D339	0 0 0 0 0	
5.623E-04	1.092E-01	25	F322	2 0 1 1 0	EFG
1.030E-03	2.000E-01	25	O027	1 0 1 0 0	
7.465E-04	1.450E-01	25	P013	0 0 0 0 0	
1.200E-03	2.331E-01	27	B129	2 2 2 2 1	
1.200E-03	2.331E-01	27	G078	2 1 0 1 0	EFG
1.777E-03	3.452E-01	30	A059	1 0 1 1 1	
2.221E-03	4.314E-01	35	A059	1 0 1 1 1	
2.064E-03	4.009E-01	39.3	G302	2 2 2 2 0	EFG
2.610E-03	5.069E-01	40	A059	1 0 1 1 1	
7.155E-04	1.390E-01	ns	B404	0 2 1 1 0	
1.100E-03	2.137E-01	ns	G067	2 0 1 1 1	
9.989E-04	1.940E-01	rt	I404	0 0 0 0 0	Intrinsic, Average

2472. C₁₁H₁₄O₃

4-Methoxyphenylbutyric acid

RN: 4521-28-2 **MP (°C):** 57
MW: 194.23 **BP (°C):** 335

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.122E+00	9.949E+02	37	A407	2 2 2 2 2	

2473. C₁₁H₁₄O₄

Dimethyl carbate
Dimelone

RN: 5826-73-3 **MP (°C):** 38
MW: 210.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-02	1.303E+01	35	M061	1 0 0 0 2	

2474. C₁₁H₁₅BrClO₃PS

Profenofos
O-(4-Bromo-2-chlorophenyl)-O-ethyl-S-propyl phosphorothioate
Selecron
Curacron
Polycron

RN: 41198-08-7 **MP (°C):**
MW: 373.64 **BP (°C):** 110

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.353E-05	2.000E-02	20	E048	1 2 1 1 1	
5.353E-05	2.000E-02	20	M161	1 0 0 0 1	
7.499E-05	2.802E-02	ns	S460	0 0 0 0 0	

2475. C₁₁H₁₅BrN₂O

Butallylonal
5-(2-Bromoallyl)-5-sec-butylbarbituric acid
Dial
RN: 1142-70-7 **MP (°C):** 131.5
MW: 271.16 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.522E-03	6.840E-01	ns	T003	0 0 0 0 2	

2476. C₁₁H₁₅FN₂O₄

1-Hexyloxycarbonyl-5-fluorouracil
1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, hexyl ester
RN: 66999-99-3 **MP (°C):** 68
MW: 258.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.808E-03	1.500E+00	22	B332	1 1 0 0 1	pH 4.0

2477. C₁₁H₁₅NO₂

m-Isopropylphenyl *N*-methylcarbamate
 3-Isopropylphenyl *N*-methylcarbamate
 UC-10854

RN: 64-00-6 **MP (°C):** 53
MW: 193.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.398E-04	8.500E-02	30	D089	2 2 0 0 0	
4.398E-04	8.500E-02	30	M061	1 0 0 0 1	

2478. C₁₁H₁₅NO₂

Butamben
 4-Aminobenzoic acid butyl ester
 Butyl *p*-aminobenzoate

RN: 94-25-7 **MP (°C):** 58.0
MW: 193.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-03	1.990E-01	25	H008	0 0 0 0 0	
8.332E-04	1.610E-01	25	P303	0 0 0 0 0	
1.200E-03	2.319E-01	30	J018	1 2 0 1 1	0.05N NaOH
1.200E-03	2.319E-01	30	J022	1 0 2 1 1	
1.200E-03	2.319E-01	30	N045	1 2 2 2 0	EFG
1.389E-03	2.683E-01	33	P303	0 0 0 0 0	
1.720E-03	3.324E-01	37	F006	1 1 2 2 2	
1.700E-03	3.285E-01	37	J026	2 2 2 1 1	
2.221E-03	4.293E-01	40	P303	0 0 0 0 0	
6.468E-04	1.250E-01	ns	B404	0 2 1 1 0	
7.140E-04	1.380E-01	ns	M066	0 0 0 0 2	
7.140E-04	1.380E-01	rt	B016	0 0 1 1 2	pH 7.4
7.784E-04	1.504E-01	rt	I404	0 0 0 0 0	Average

2479. C₁₁H₁₅NO₂S

Ethiocencarb
 2-((Ethylthio)methyl)phenyl methylcarbamate
 Ethylmercaptopethylphenyl-*N*-methylcarbamate
 Ethiophencarp

Croneton

HOX 1901

RN: 29973-13-5 **MP (°C):** <25
MW: 225.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.078E-03	1.820E+00	20	M161	1 0 0 0 2	

2480. C₁₁H₁₅NO₃ $\alpha,3$ -*o*-Isopropylidene pyriridoxine

RN: MP (°C):

MW: 209.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.196E-02	2.503E+00	37	M067	2 0 1 1 2	

2481. C₁₁H₁₅NO₃

Propoxur

o-Isopropoxyphenyl methylcarbamate

Baygon

Blattanex

Blattosep

Suncide

RN: 114-26-1 MP (°C): 91

MW: 209.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.301E-03	1.737E+00	10	B324	0 0 0 0 0	
8.316E-03	1.740E+00	10	B324	0 0 0 0 0	
8.885E-03	1.859E+00	20	B300	2 2 1 1 2	
9.244E-03	1.934E+00	20	B324	0 0 0 0 0	
9.206E-03	1.926E+00	20	B324	0 0 0 0 0	
9.558E-03	2.000E+00	20	M161	1 0 0 0 0	
1.166E-02	2.440E+00	30	B324	0 0 0 0 0	
1.163E-02	2.434E+00	30	B324	0 0 0 0 0	
4.732E-02	9.901E+00	ns	M061	0 0 0 0 0	approximate
4.301E-04	9.000E-02	ns	M110	0 0 0 0 0	EFG

2482. C₁₁H₁₅NO₄*n*-Ethyl-6-hydroxynorbornane-2-carboxamide-3,5-lactone

RN: MP (°C):

MW: 225.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.908E-01	6.550E+01	20	K050	1 1 1 1 2	

2483. C₁₁H₁₅N₃O₂

Formetanate

Methylcarbamic acid, ester with *N'*-(*m*-hydroxyphenyl)-*N,N*-dimethylformamidine

RN: 22259-30-9 MP (°C): 102.5

MW: 221.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.520E-03	1.000E+00	rt	M161	0 0 0 0 0	

2484. C₁₁H₁₅N₃O₃

Orotic acid cyclohexylamide
Orotamide, *N*-cyclohexyl-

RN: 4558-58-1 **MP (°C):** 284–285
MW: 237.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.500E-02	1.779E+01	–4	N018	0 0 0 0 0	
1.100E-01	2.610E+01	16	N018	0 0 0 0 0	
1.330E-01	3.156E+01	25	N018	0 0 0 0 0	

2485. C₁₁H₁₅N₃O₅

Triglycidylurazol
Anaxirone

RN: 77658-97-0 **MP (°C):** 91
MW: 269.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.426E-04	2.000E-01	ns	D319	0 0 0 0 0	

2486. C₁₁H₁₅O₃P

Diethyl benzoyl phosphonate
Methylene, (diethoxyphosphinyl)phenyl-

RN: 105394-75-0 **MP (°C):**
MW: 226.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<8.84E-04	<2.00E-01	25	B070	1 2 0 1 0	

2487. C₁₁H₁₆

tert-Amylbenzene
t-Amylbenzene

RN: 2049-95-8 **MP (°C):** –57.8
MW: 148.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.083E-05	1.050E-02	25	A002	1 2 1 1 2	

2488. C₁₁H₁₆

Amylbenzene

n-Pentylbenzene

Pentylbenzene

n-Amylbenzene*n*-Pentylbenzene1-phenylpentane

RN: 538-68-1 **MP (°C):** -75
MW: 148.25 **BP (°C):** 205.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E-05	3.481E-03	7	O312	2 2 0 2 2	
2.144E-05	3.178E-03	10	O312	2 2 0 2 2	
2.323E-05	3.444E-03	12.5	O312	2 2 0 2 2	
2.153E-05	3.192E-03	15	O312	2 2 0 2 2	
2.311E-05	3.426E-03	17.5	O312	2 2 0 2 2	
2.142E-05	3.176E-03	20	O312	2 2 0 2 2	
2.590E-05	3.840E-03	25	M342	1 0 1 1 2	
2.276E-05	3.374E-03	25	O312	2 2 0 2 2	
2.433E-05	3.607E-03	30	O312	2 2 0 2 2	
2.642E-05	3.917E-03	35	O312	2 2 0 2 2	
2.868E-05	4.252E-03	40	O312	2 2 0 2 2	
3.163E-05	4.689E-03	45	O312	2 2 0 2 2	
6.000E-03	8.895E-01	ns	H307	0 0 0 0 0	

2489. C₁₁H₁₆

Pentamethylbenzene

1,2,3,4,5-Pentamethyl benzene

RN: 700-12-9 **MP (°C):** 50.8
MW: 148.25 **BP (°C):** 231.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-04	1.552E-02	ns	D001	0 0 0 0 2	

2490. C₁₁H₁₆ClO₂PS₃

Carbophenothon

O,O-Diethyl *S*-(4-chlorophenylthiomethyl) dithiophosphate

Trithion

Garrathion

Nephocarp

Lethox

RN: 786-19-6 **MP (°C):** <25
MW: 342.87 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.779E-06	6.100E-04	10	B324	0 0 0 0 0	
1.779E-06	6.100E-04	10	B324	0 0 0 0 0	
1.838E-06	6.302E-04	20	B300	2 1 1 1 2	

(continued)

2490. C₁₁H₁₆ClO₂PS₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.837E-06	6.300E-04	20	B324	0 0 0 0 0	
1.838E-06	6.302E-04	20	B324	0 0 0 0 0	
2.129E-06	7.300E-04	30	B324	0 0 0 0 0	
2.129E-06	7.300E-04	30	B324	0 0 0 0 0	
<1.17E-04	<4.00E-02	ns	M161	0 0 0 0 0	

2491. C₁₁H₁₆N₂O₂

4-Aminobenzoic acid-2-(ethyl-amino)ethyl ester

2-(Ethylamino)ethyl 4-aminobenzoate

RN: MP (°C):

MW: 208.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-02	5.623E+00	ns	M066	0 0 0 0 1	

2492. C₁₁H₁₆N₂O₂

Aminocarb

Phenol, 4-(dimethylamino)-3-methyl, methylcarbamate (ester)

Carbamic acid, methyl-, 4-(dimethylamino)-*m*-tolyl ester

RN: 2032-59-9 MP (°C): 93

MW: 208.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.187E-03	8.720E-01	10	B324	0 0 0 0 0	
4.183E-03	8.712E-01	10	B324	0 0 0 0 0	
4.394E-03	9.151E-01	20	B300	2 2 1 1 2	
4.389E-03	9.142E-01	20	B324	0 0 0 0 0	
4.394E-03	9.151E-01	20	B324	0 0 0 0 0	
4.393E-03	9.150E-01	20	G300	1 0 0 0 2	
6.521E-03	1.358E+00	30	B324	0 0 0 0 0	
6.540E-03	1.362E+00	30	B324	0 0 0 0 0	

2493. C₁₁H₁₆N₂O₃

Vinbarbital

5-Ethyl-5-(1-methyl-1-but enyl)barbituric acid

RN: 125-42-8 MP (°C): 161

MW: 224.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-03	7.000E-01	25	B011	2 0 0 1 0	
3.164E-03	7.097E-01	25	B065	1 1 1 1 1	
4.870E-03	1.092E+00	25	V033	2 0 1 1 2	

(continued)

2493. C₁₁H₁₆N₂O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	1.099E+00	25.00	T303	1 0 0 0 1	
7.000E-03	1.570E+00	35.00	T303	1 0 0 0 1	
8.000E-03	1.794E+00	45.00	T303	1 0 0 0 1	

2494. C₁₁H₁₆N₂O₃

5-Allyl-5-butylbarbituric acid

n-Butylallylbarbitone*n*-Butylallylbarbituric acid

Allylbutylbarbituric acid

Idobutal

RN: 3146-66-5 MP (°C):

MW: 224.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.723E-03	1.508E+00	20	J030	1 2 2 2 2	
8.945E-03	2.006E+00	37	J030	1 2 2 2 2	

2495. C₁₁H₁₆N₂O₃

Talbutal

Allyl-*sec*-butyl-barbituric acid5-Allyl-5-*sec*-butylbarbituric acid

RN: 115-44-6 MP (°C): 109

MW: 224.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.632E-03	2.160E+00	ns	T003	0 0 0 0 2	

2496. C₁₁H₁₆N₂O₃

Butalbital

Itobarbital

5-Allyl-5-isobutylbarbituric acid

Fioricet

Phrenilin

Medigesic

RN: 77-26-9 MP (°C): 138

MW: 224.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.590E-03	1.702E+00	25	V033	2 0 1 1 2	
7.600E-03	1.704E+00	25.00	T303	1 0 0 0 1	
1.030E-02	2.310E+00	35.00	T303	1 0 0 0 2	
1.410E-02	3.162E+00	45.00	T303	1 0 0 0 2	

2497. C₁₁H₁₆N₂O₃

2,4-Diazaspiro[5.7]tridecane-1,3,5-trione

RN: 143288-62-4 MP (°C):

MW: 224.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.042E-03	2.337E-01	25	P350	0 0 0 0 0	intrinsic

2498. C₁₁H₁₆N₂O₃

Barbituric acid, 5-ethyl-5-(3-methyl-2-butenyl)

5-Ethyl-5-(3'-methylbut-2'-enyl)barbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methyl-2-butenyl)-

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-(3-methyl-2-butenyl)-

5-Ethyl-5-(3-methylbut-2-enyl)barbiturate

RN: 21149-88-2 MP (°C):

MW: 224.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.583E-03	1.252E+00	25	P350	0 0 0 0 0	intrinsic

2499. C₁₁H₁₆N₂O₃S

Phenbutamide

N-(Phenylsulfonyl)-N'-butylurea

N-Benzene sulfonyl-N'-n-butylurea

RN: 3149-00-6 MP (°C): 131

MW: 256.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.995E-04	2.306E-01	37	A028	1 0 2 1 2	intrinsic
9.000E-04	2.307E-01	37	A046	2 0 1 1 2	

2500. C₁₁H₁₆N₂O₄

Methyl-2-ethyl-2-allylmalonurate

Methyl 2-ethyl-2-allylmalonurate

RN: 73632-83-4 MP (°C): 78.5

MW: 240.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	2.883E+00	23	B152	1 2 1 1 1	pH 3.5

2501. C₁₁H₁₆N₂O₅

Methoxycarbonylmethyl-2,2-diethylmalonurate
Methoxycarbonylmethyl 2,2-diethylmalonurate

RN: **MP (°C):** 89
MW: 256.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-03	2.486E+00	23	B152	1 2 1 1 1	pH 3.5

2502. C₁₁H₁₆N₄O₂

1-Butyl theobromine
1-Butyl-3,7-dimethylxanthine
1-n-Butyl-3,7-dimethylxanthine

RN: 1143-30-2 **MP (°C):** 108
MW: 236.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.370E-02	5.600E+00	30	B042	1 2 1 1 2	

2503. C₁₁H₁₆N₄O₄

2,6-Piperazinedione, 4,4'-(1-methyl-1,2-ethanediyl)bis-
1,2-Di(4-piperazine-2,6-dione)propane
2,6-Piperazinedione, 4,4'-(1-methyl-1,2-ethanediyl)bis-, (\pm)-, polymer with 1,3-dibromopropane
Propane, 1,3-dibromo-, polymer with (\pm)-4,4'-(1-methyl-1,2-ethanediyl)bis[2,6-piperazinedione]

RN: 21416-67-1 **MP (°C):** 192 dec
MW: 268.27 **BP (°C):** 233 dec

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.118E-02	3.000E+00	25	P326	0 0 0 0 0	
~5.59E-02	~1.50E+01	25	R017	0 0 0 0 0	enantiomer (R)
~1.12E-02	~3.00E+00	25	R017	0 0 0 0 0	

2504. C₁₁H₁₆O

p-sec-Amylphenol
4-sec-Amylphenol

RN: 25735-67-5 **MP (°C):**
MW: 164.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.408E-04	1.053E-01	25	L021	1 0 0 0 0	

2505. C₁₁H₁₆O*p-n*-Amylphenol4-*n*-Pentylphenol

RN: 14938-35-3 **MP (°C):**
MW: 164.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.088E-04	9.999E-02	25	L022	1 0 0 0 0	

2506. C₁₁H₁₆O*p-tert*-Pentylphenol*p-(α,α-Dimethylpropyl)phenol**p-(1,1-Dimethylpropyl)phenol*

1-Hydroxy-4(2-methyl-2-butyl)benzene

PTAP

RN: 80-46-6 **MP (°C):**
MW: 164.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.162E-04	1.176E-01	25	L021	1 0 0 0 0	
1.023E-03	1.680E-01	25	M127	1 0 0 0 2	

2507. C₁₁H₁₆O

4-(1,1-Dimethylethyl)benzenemethanol

4-(1,1-Dimethylethyl)benzyl alcohol

4-*tert*-Butylbenzyl alcohol4-*tert*-Butylphenylmethanol*p-tert*-Butylbenzyl alcohol

RN: 877-65-6 **MP (°C):**
MW: 164.25 **BP (°C):** 250.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-03	1.051E+00	20	B407	1 0 1 2 2	

2508. C₁₁H₁₆O*o-n*-Amylphenol2-*n*-Amylphenol

RN: 87-26-3 **MP (°C):**
MW: 164.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.365E-04	1.538E-01	25	L022	1 0 0 0 0	

2509. C₁₁H₁₆O

o-2-Hexenylphenol

2-2-Hexenylphenol

RN: 75121-79-8 MP (°C):

MW: 164.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.162E-04	1.176E-01	25	L021	1 0 0 0 0	

2510. C₁₁H₁₆O2-Methyl-5-*t*-butylphenol5-*tert*-Butyl-2-methylphenol5-*tert*-Butyl-*o*-cresol*o*-Cresol, 5-*tert*-butyl-

RN: 5781-02-2 MP (°C):

MW: 164.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.533E-03	4.160E-01	25	M127	1 0 0 0 2	

2511. C₁₁H₁₆O₂4-*n*-Amyl resorcinol4-*n*-Amyl-resorcin

RN: 533-24-4 MP (°C):

MW: 180.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-02	2.000E+00	20	F300	1 0 0 0 0	

2512. C₁₁H₁₆O₂

3-Pentoxyphenol

m-Pentoxy phenol

Phenol, 3-pentoxy-

RN: 18979-73-2 MP (°C):

MW: 180.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.130E-03	3.839E-01	30	B315	0 0 0 0 0	

2513. C₁₁H₁₇NO₃

Dimetan

5,5-Dimethyldihydroresorcinyl N,N-dimethylcarbamate

RN: 122-15-6 MP (°C): 45.5

MW: 211.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	2.913E+01	ns	M061	0 0 0 0 0	approximate

2514. C₁₁H₁₇N₃O₃

Orotic acid triethylamide

RN: MP (°C): 200–202

MW: 239.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.261E+00	5.410E+02	25	N018	0 0 0 0 0	

2515. C₁₁H₁₇N₃O₃S

Carbutamide

4-Amino-N-[(butylamino)carbonyl]-benzenesulfonamide

1-Butyl-3-sulfanilyl urea

RN: 339-43-5 MP (°C): 144.5

MW: 271.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.972E-03	5.352E-01	37	A028	1 0 2 1 2	intrinsic
1.950E-03	5.291E-01	37	A046	2 0 1 1 2	
6.634E-03	1.800E+00	37	C054	2 0 2 1 2	0.1N HCl

2516. C₁₁H₁₇N₃O₆

Orotic acid triethanolamide

RN: MP (°C): 104–108

MW: 287.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E+00	3.778E+02	-4	N018	0 0 0 0 0	
1.882E+00	5.407E+02	16	N018	0 0 0 0 0	
2.187E+00	6.283E+02	25	N018	0 0 0 0 0	

2517. C₁₁H₁₇O₃PS

Kitazin

O,O-Diethyl *S*-benzyl thiophosphate

EBP

S-Benzyl *O,O*-di-ethyl phosphorothioate

RN: 13286-32-3 **MP (°C):**
MW: 260.29 **BP (°C):** 115

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.537E-03	4.000E-01	22	K137	1 1 2 1 0	

2518. C₁₁H₁₇O₃PS₂

Fensulfothion sulfide

O,O-Diethyl *O*-[*p*-(methylthio)phenyl] phosphorothioatePhosphorothioic acid, *O,O*-diethyl *O*-[4-(methylthio)phenyl] ester

RN: 3070-15-3 **MP (°C):**
MW: 292.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.266E-05	3.700E-03	20	M318	2 2 0 0 2	

2519. C₁₁H₁₇O₄PS₂

Fensulfothion

O,O-Diethyl *O*-(4-(methylsulfinyl)phenyl) phosphorothioate

Dasanit

Bay 25141

Agricur

Chemagro 25141

RN: 115-90-2 **MP (°C):** <25
MW: 308.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.473E-03	1.996E+00	20	B169	2 2 1 1 2	
6.473E-03	1.996E+00	20	F318	2 2 0 0 2	
4.994E-03	1.540E+00	25	M161	1 0 0 0 2	

2520. C₁₁H₁₇O₅PS₂

Fensulfothion sulfone

Phosphorothioic acid, *O,O*-diethyl *O*-[*p*-(methylsulfonyl)phenyl] ester

Dasanit sulfone

Dasanit sulphone

RN: 14255-72-2 MP (°C):

MW: 324.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.242E-04	4.030E-02	10	B324	0 0 0 0 0	
1.243E-04	4.032E-02	10	B324	0 0 0 0 0	
2.300E-04	7.459E-02	20	B169	2 2 1 1 2	
2.633E-04	8.540E-02	20	B324	0 0 0 0 0	
2.633E-04	8.539E-02	20	B324	0 0 0 0 0	
2.300E-04	7.459E-02	20	M318	2 2 0 0 2	
3.576E-04	1.160E-01	30	B324	0 0 0 0 0	
3.576E-04	1.160E-01	30	B324	0 0 0 0 0	

2521. C₁₁H₁₈N₂O₂S

Thiopental

5-Ethyl-5-(1-methyl-butyl)-2-thiobarbituric acid

5-Ethyl-5-(1-methylbutyl)-2-thiobarbituric acid

Barbituric acid, 5-ethyl-5-(1-methylbutyl)-2-thio

4,6(1H,5H)-Pyrimidinedione, 5-ethyldihydro-5-(1-methylbutyl)-2-thioxo

Pentothiobarbital

RN: 76-75-5 MP (°C): 158

MW: 242.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.063E-04	5.000E-02	25	A023	1 0 0 1 1	
3.301E-04	8.000E-02	25	B011	2 0 0 1 0	
3.333E-04	8.077E-02	25	B065	1 1 1 1 1	
8.200E-04	1.987E-01	25	G003	1 1 1 1 1	pH 4.7
2.094E-04	5.075E-02	25	P350	0 0 0 0 0	intrinsic
3.000E-04	7.270E-02	30	K108	1 2 2 0 0	
3.301E-04	7.999E-02	35	A023	1 0 0 1 1	
4.126E-04	9.999E-02	40	A023	1 0 0 1 1	

2522. C₁₁H₁₈N₂O₃

Amobarbital

5-Ethyl-5-isoamylbarbituric acid

Amylobarbitone

RN: 57-43-2**MP (°C):** 157**MW:** 226.28**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.828E-03	6.400E-01	20	J030	1 2 2 2 1	
3.533E-03	7.994E-01	25	A023	1 0 0 1 1	
2.475E-03	5.600E-01	25	B011	2 0 0 1 0	
2.665E-03	6.030E-01	25	B065	1 1 1 1 1	
3.900E-03	8.825E-01	25	G003	1 1 1 1 1	pH 4.7
2.170E-03	4.910E-01	25	V033	2 0 1 1 2	
2.200E-03	4.978E-01	25.00	T303	1 0 0 0 1	
3.000E-03	6.788E-01	30	G014	1 1 1 1 0	EFG
3.100E-03	7.015E-01	30	I001	2 0 2 1 0	EFG, 0.003N H ₂ SO ₄
2.846E-03	6.440E-01	30	I015	1 2 2 1 2	pH 6.0, 3 forms
3.200E-03	7.241E-01	30	K108	1 2 2 0 1	
3.300E-03	7.467E-01	35.00	T303	1 0 0 0 1	
4.375E-03	9.900E-01	37	J030	1 2 2 2 1	
4.000E-03	9.051E-01	37	K121	1 2 1 2 0	0.1N HCl
5.517E-03	1.248E+00	40	A023	1 0 0 1 1	
3.820E-02	8.644E+00	40	N008	1 0 1 1 2	sic
4.300E-03	9.730E-01	45.00	T303	1 0 0 0 1	
2.342E-03	5.300E-01	ns	T003	0 0 0 0 2	

2523. C₁₁H₁₈N₂O₃

Pentobarbital

5-ethyl-5-(1-methyl-butyl)-barbituric acid

RN: 76-74-4**MP (°C):** 130**MW:** 226.28**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.415E-03	9.990E-01	25	A023	1 0 0 1 1	
2.210E-03	5.000E-01	25	B011	2 0 0 1 0	
2.221E-03	5.026E-01	25	B065	1 1 1 1 1	
3.000E-03	6.788E-01	25	G003	1 1 1 1 1	pH 4.7
4.070E-03	9.210E-01	25	V033	2 0 1 1 2	
4.100E-03	9.277E-01	25.00	T303	1 0 0 0 1	
6.000E-03	1.358E+00	30	K108	1 2 2 0 1	
6.178E-03	1.398E+00	35	A023	1 0 0 1 1	
5.700E-03	1.290E+00	35.00	T303	1 0 0 0 1	
7.000E-03	1.584E+00	37	K121	1 2 1 2 0	0.1N HCl
7.060E-03	1.597E+00	40	A023	1 0 0 1 1	
7.640E-02	1.729E+01	40	N008	1 0 1 1 2	sic
6.900E-03	1.561E+00	45.00	T303	1 0 0 0 1	
4.365E-03	9.877E-01	ns	R427	0 0 0 0 0	

2524. C₁₁H₁₈N₂O₃

5-n-Pentyl-5-ethylbarbituric acid

5-Ethyl-5-pentylbarbituric acid

5-Ethyl-5-pentylbarbiturate

RN: 115-58-2 **MP (°C):** 135.5**MW:** 226.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.657E-03	1.506E+00	25	B065	1 2 1 1 1	
2.448E-03	5.540E-01	ns	T003	0 0 0 0 2	

2525. C₁₁H₁₈N₂O₃

Pilocarpic acid

1,2-Secopilocarpin-2-oic acid

RN: 28406-15-7 **MP (°C):****MW:** 226.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.303E-04	1.200E-01	23	B340	1 1 2 1 1	pH 9

2526. C₁₁H₁₈N₄O₂

Pirimicarb

2-(Dimethylamino)-5,6-dimethyl-4-pyrimidinyl dimethylcarbamate

Abol

Rapid

Fernos

Aphox

RN: 23103-98-2 **MP (°C):** 90.5**MW:** 238.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.133E-02	2.700E+00	25	M161	1 0 0 0 1	

2527. C₁₁H₁₉N₃O

Dimethirimol

2-Dimethylamino-4-hydroxy-5-n-butyl-6-methylpyrimidine

RN: 5221-53-4 **MP (°C):** 102**MW:** 209.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.734E-03	1.200E+00	25	M161	1 0 0 0 1	
5.727E-03	1.199E+00	ns	M061	0 0 0 0 1	

2528. C₁₁H₁₉N₃O

Ethirimol

5-Butyl-2-(ethylamino)-4-hydroxy-6-methylpyrimidine

Milgo

Milcurl super

Milstem

RN: 23947-60-6 **MP (°C):** 159.5
MW: 209.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.556E-04	2.000E-01	rt	M161	0 0 0 0 0	

2529. C₁₁H₂₀

2-Methyldecalin

Decahydro-2-methylnaphthalene

RN: 2958-76-1 **MP (°C):**
MW: 152.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.666E-07	4.060E-05	25	B069	1 0 1 1 2	

2530. C₁₁H₂₀ClN₅

Chlorazine

2-Chloro-4-diethylamino-6-diethylamino-s-triazine

2-Chloro-4,6-*bis*-(diethylamino)-s-triazine chlorazine

1,3,5-Triazine

1,3,5-Triazine-2,4-diamine

RN: 580-48-3 **MP (°C):**
MW: 257.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.492E-05	9.000E-03	20	J033	0 0 0 0 0	
3.879E-05	1.000E-02	21	B192	0 0 0 0 1	
3.492E-05	9.000E-03	21	G099	2 0 0 1 0	

2531. C₁₁H₂₀N₂O₄

Isopropyl-2,2-diethylmalonurate

Isopropyl 2,2-diethylmalonurate

RN: 73632-77-6 **MP (°C):** 99.5
MW: 244.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-03	4.153E-01	23	B152	1 2 1 1 1	pH 3.5

2532. C₁₁H₂₀N₃O₃PS

Pirimiphos-methyl

Pirimiphosmethyl

RN: 29232-93-7 MP (°C): 15

MW: 305.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.139E-05	2.180E-02	10	B324	0 0 0 0 0	
7.946E-05	2.426E-02	10	B324	0 0 0 0 0	
7.363E-05	2.248E-02	20	B300	2 1 1 1 2	
1.119E-04	3.417E-02	20	B324	0 0 0 0 0	
1.005E-04	3.070E-02	20	B324	0 0 0 0 0	
1.640E-04	5.008E-02	30	B324	0 0 0 0 0	
1.474E-04	4.500E-02	30	B324	0 0 0 0 0	
1.638E-05	5.000E-03	30	M161	1 0 0 0 0	sic

2533. C₁₁H₂₀N₆1-(Pyrrolidinyl)-3,5-bis(dimethylamino)-*s*-triazine1-Pyrrolidino-3,5-bis(dimethylamino)-*s*-triazine

RN: 13452-85-2 MP (°C):

MW: 236.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-04	3.878E-02	25	B386	0 0 0 0 0	

2534. C₁₁H₂₀N₆O1-(Morpholinyl)-3,5-bis(dimethylamino)-*s*-triazine*s*-Triazine, 2,4-bis(dimethylamino)-6-morpholino-

RN: 16269-02-6 MP (°C):

MW: 252.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.303E-03	3.288E-01	25	B386	0 0 0 0 0	

2535. C₁₁H₂₀N₆S1-(Thiomorpholinyl)-3,5-bis(dimethylamino)-*s*-triazine1,3,5-Triazine-2,4-diamine, *N,N,N',N'*-tetramethyl-6-(4-thiomorpholinyl)-

RN: 41492-69-7 MP (°C):

MW: 268.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.689E-05	1.527E-02	25	B386	0 0 0 0 0	

2536. C₁₁H₂₀O₂

Undecylenic acid

10-Undecylenic acid

Hendecenoic acid

RN: 112-38-9

MP (°C): 25

MW: 184.28

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	7.371E-02	30	D051	2 0 0 1 2	
1.074E-04	1.980E-02	30	E005	2 1 1 2 2	
1.248E-04	2.300E-02	40	E005	2 1 1 2 1	
1.411E-04	2.600E-02	50	E005	2 1 1 2 1	
1.000E-03	1.843E-01	60	D051	2 0 0 1 2	
1.736E-04	3.200E-02	60	E005	2 1 1 2 1	

2537. C₁₁H₂₀O₄

Hexyl α-acetoxypropionate

Propanoic acid, 2-(acetyloxy)-, hexyl ester

RN: 96884-73-0 MP (°C):

MW: 216.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.247E-04	2.000E-01	25	R006	2 2 0 1 1	

2538. C₁₁H₂₀O₄

Undecanedioic acid

1,9-Nonanedicarboxylic acid

Nonan-dicarbonsaeure-(1,9)

RN: 1852-04-6 MP (°C):

MW: 216.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.358E-02	5.100E+00	21	B040	1 0 1 1 1	<i>sic</i>
6.473E-04	1.400E-01	ns	F300	0 0 0 0 2	

2539. C₁₁H₂₀O₅

Propanoic acid, 2-[(hexthoxycarbonyl)oxy]-, methyl ester

RN: MP (°C):

MW: 232.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.305E-04	9.999E-02	25	R007	0 0 0 0 0	

2540. C₁₁H₂₁BrO₂

11-Bromoundecanoic acid

Bromo-11-undecanoic acid

RN: 2834-05-1 **MP (°C):** 49.5
MW: 265.20 **BP (°C):** 173.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	5.304E-02	30	D051	2 0 0 1 2	
7.500E-04	1.989E-01	60	D051	2 0 0 1 2	

2541. C₁₁H₂₁NOS

Cycloate

S-Ethyl N-ethylthiocyclohexanecarbamate

RO-Neet

S-Ethyl N,N-ethylcyclohexylthiocarbamate

RN: 1134-23-2 **MP (°C):** 12
MW: 215.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.947E-04	8.500E-02	22	B200	1 0 0 0 1	
3.947E-04	8.500E-02	22	F019	1 0 0 0 1	
3.947E-04	8.500E-02	22	M161	1 0 0 0 1	

2542. C₁₁H₂₁NO₃

Dipropylaceturethane

RN: **MP (°C):**
MW: 215.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.857E-03	3.998E-01	20	O021	1 2 0 0 0	

2543. C₁₁H₂₁N₅O

Ipatone

1,3,5-Triazine, 2-(diethylamino)-4-(isopropylamino)-6-methoxy

1,3,5-Triazine-2,4-diamine, *N,N*-diethyl-6-methoxy-*N'*-(1-methylethyl)

RN: 3004-70-4 **MP (°C):**
MW: 239.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.178E-04	1.000E-01	20	J033	0 0 0 0 0	

2544. C₁₁H₂₁N₅OS

Gesaran

2-Methylthio-4-isopropylamino-6-(3-methoxypropylamino)-*s*-triazine

Methoprotyne

RN: 841-06-5 **MP (°C):** 69**MW:** 271.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.179E-03	3.200E-01	20	F311	1 2 2 2 1	
1.179E-03	3.200E-01	20	M161	1 0 0 0 2	
1.179E-03	3.200E-01	ns	J033	0 0 0 0 0	
3.681E-03	9.990E-01	ns	M061	0 0 0 0 0	

2545. C₁₁H₂₁N₅S

Dimethametryn

N-(1,2-Dimethylpropyl)-*N'*-ethyl-6-(methylthio)-1,3,5-triazine-2,4-diamine

Belclene 310

RN: 22936-75-0 **MP (°C):****MW:** 255.39 **BP (°C):** 152

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.958E-04	5.000E-02	20	M161	1 0 0 0 1	

2546. C₁₁H₂₁N₅S

Dipropetryn

2-(Ethylthio)-4,6-bis(isopropylamino)-*s*-triazine

Cotofor

Sancap

Sancap 80W

RN: 4147-51-7 **MP (°C):** 105**MW:** 255.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.265E-05	1.600E-02	rt	M161	0 0 0 0 1	

2547. C₁₁H₂₁N₅S

Ipatryne

2-Methylmercapto-4-isopropylamino-6-diethylamino-*s*-triazine**RN:** **MP (°C):****MW:** 255.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-05	5.363E-03	26	G001	1 0 1 1 1	

2548. C₁₁H₂₁N₇

1-(1-Piperazinyl)-3,5-bis(dimethylamino)-*s*-triazine
 1,3,5-Triazine-2,4-diamine, *N,N,N',N'*-tetramethyl-6-(1-piperazinyl)-

RN: 125867-94-9 **MP (°C):**
MW: 251.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.081E-02	2.717E+00	25	B386	0 0 0 0 0	

2549. C₁₁H₂₁O₅

Propanoic acid, 2-[(proxycarbonyl)oxy]-, butyl ester

RN: **MP (°C):**
MW: 233.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.286E-04	9.999E-02	25	R007	0 0 0 0 0	

2550. C₁₁H₂₂N₂O

Cycluron

N'-Cyclooctyl-*N,N*-dimethylurea

Cyclooctyl-1,1-dimethylurea

OMU

RN: 2163-69-1 **MP (°C):** 138
MW: 198.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.564E-04	1.500E-01	20	B185	0 0 0 0 0	
6.051E-03	1.200E+00	20	G036	1 0 0 0 2	
5.541E-03	1.099E+00	20	M061	1 0 0 0 1	
5.547E-03	1.100E+00	20	M161	1 0 0 0 1	
6.310E-04	1.251E-01	ns	M163	0 0 0 0 0	EFG

2551. C₁₁H₂₂N₆

*N*6,*N*6-Diethyl-*N*2,*N*2,*N*4,*N*4-tetramethylmelamine

1,3,5-Triazine-2,4,6-triamine, *N,N*-diethyl-*N'*,*N'*,*N''*,*N''*-tetramethyl-

RN: 16268-75-0 **MP (°C):** 42.0
MW: 238.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.979E-04	7.100E-02	25	C051	1 2 1 1 1	pH 7

2552. C₁₁H₂₂O₂

Undecanoic acid

Undecanoique acide

RN: 112-37-8

MP (°C): 28.5

MW: 186.30

BP (°C): 228

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.382E-03	6.300E-01	0	B136	1 0 2 1 1	
5.744E-04	1.070E-01	20	B136	1 0 2 1 2	
4.992E-04	9.299E-02	20.0	R001	1 1 1 1 1	
6.978E-04	1.300E-01	30	B136	1 0 2 1 2	
2.800E-04	5.216E-02	30	D051	2 0 0 1 2	
5.904E-04	1.100E-01	30.0	R001	1 1 1 1 1	
7.730E-04	1.440E-01	40	B136	1 0 2 1 2	
6.978E-04	1.300E-01	45	B136	1 0 2 1 1	
6.977E-04	1.300E-01	45.0	R001	1 1 1 1 1	
8.052E-04	1.500E-01	60	B136	1 0 2 1 1	
6.000E-04	1.118E-01	60	D051	2 0 0 1 2	
8.050E-04	1.500E-01	60.0	R001	1 1 1 1 1	
3.381E-04	6.300E-02	.0	R001	1 1 1 1 1	

2553. C₁₁H₂₂O₂

Methyl caprate

Capric acid methyl ester

Methyl decanoate

RN: 110-42-9

MP (°C): -13

MW: 186.30

BP (°C): 223

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.36E-05	<4.40E-03	20	M337	2 1 2 2 1	
2.051E-05	3.821E-03	ns	S460	0 0 0 0 0	

2554. C₁₁H₂₂O₂

Ethyl nonanoate

Ethyl nonylate

RN: 123-29-5

MP (°C):

MW: 186.30

BP (°C): 119 at 23 mm

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-04	2.953E-02	ns	S460	0 0 0 0 0	

2555. C₁₁H₂₂O₂

3-Hydroxy-2-propyl-5,5-diethyltetrahydrofuran

RN: MP (°C):

MW: 186.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.053E-01	1.961E+01	rt	B066	0 2 0 0 0	

2556. C₁₁H₂₂O₃*n*-Hexyl β-ethoxypropionate

Propionic acid, 3-ethoxy-, hexyl ester

RN: 14144-37-7 MP (°C):

MW: 202.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.483E-03	2.999E-01	25	D002	1 2 1 1 0	

2557. C₁₁H₂₂O₃

1,3-Dioxolane-4-methanol, 2-hexyl-2-methyl

2-Octanone, cyclic (hydroxymethyl)ethylene acetal

RN: 5660-52-6 MP (°C):

MW: 202.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	2.751E+00	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

2558. C₁₁H₂₂O₃

Octyl lactate

Propanoic acid, 2-hydroxy-, octyl ester

RN: 5464-71-1 MP (°C):

MW: 202.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.955E-03	8.000E-01	25	R006	2 2 0 1 0	

2559. C₁₁H₂₂O₃*n*-Butyl β-*n*-butoxypropionate

Butyl 3-butoxypropionate

Propanoic acid, 3-butoxy-, butyl ester

RN: 14144-48-0 MP (°C):

MW: 202.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.951E-03	7.994E-01	25	R034	0 0 0 0 0	

2560. C₁₁H₂₂O₄

1,3-Dioxolane-4-methanol, 2-(2-butoxyethyl)-2-methyl

RN: 143458-55-3 MP (°C):

MW: 218.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.640E-01	5.763E+01	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

2561. C₁₁H₂₃NOS

Butylate

S-Ethyl diisobutylthiocarbamate

RN: 2008-41-5 MP (°C): <25

MW: 217.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.070E-04	4.500E-02	22	B200	1 0 0 0 1	
2.070E-04	4.500E-02	22	F019	1 0 0 0 1	
1.656E-04	3.599E-02	ns	S460	0 0 0 0 0	
2.070E-04	4.500E-02	rt	M161	0 0 0 0 1	

2562. C₁₁H₂₃NO₂

11-Aminoundecanoic acid

Amino-11-undecanoic acid

RN: 2432-99-7 MP (°C): 191

MW: 201.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.986E-03	3.998E-01	20	E039	2 0 1 1 1	smoothed
1.600E-03	3.221E-01	30	D051	2 0 0 1 2	
4.962E-03	9.990E-01	30	E039	2 0 1 1 2	smoothed
8.925E-03	1.797E+00	40	E039	2 0 1 1 2	smoothed
1.486E-02	2.991E+00	50	E039	2 0 1 1 2	smoothed
1.000E-02	2.013E+00	60	D051	2 0 0 1 2	
2.471E-02	4.975E+00	60	E039	2 0 1 1 2	smoothed
3.453E-02	6.951E+00	65	E039	2 0 1 1 2	smoothed
4.431E-02	8.920E+00	70	E039	2 0 1 1 2	smoothed
5.405E-02	1.088E+01	75	E039	2 0 1 1 2	smoothed
6.858E-02	1.381E+01	80	E039	2 0 1 1 2	smoothed
8.183E-02	1.647E+01	85	E039	2 0 1 1 2	smoothed
9.740E-02	1.961E+01	90	E039	2 0 1 1 2	smoothed
1.145E-01	2.306E+01	95	E039	2 0 1 1 2	smoothed
1.259E-01	2.534E+01	100	E039	2 0 1 1 2	smoothed

2563. C₁₁H₂₄

Undecane

n-Undecane*n*-Hendecane

RN: 1120-21-4 **MP (°C):** -26
MW: 156.31 **BP (°C):** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<9.60E-06	<1.50E-03	20	M337	2 1 2 2 1	
2.815E-08	4.400E-06	25	M003	1 0 2 2 1	
5.758E-08	9.000E-06	25	T423	0 0 0 0 0	

2564. C₁₂HCl₇O

1,2,3,4,6,7,8-Heptachlorodibenzofuran

1,2,3,4,6,7,8-HpCDF

PCDF 131

F 131

RN: 67562-39-4 **MP (°C):** 236
MW: 409.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.310E-12	1.355E-09	22.5	F314	1 1 0 2 2	

2565. C₁₂HCl₇O₂1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin

1,2,3,4,6,7,8-HpCDD

PCDD 73

D 73

Heptachlorodibenzo-*p*-dioxin

RN: 35822-46-9 **MP (°C):** 265
MW: 425.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-12	9.357E-10	7.0	F315	1 2 0 2 2	
2.690E-12	1.144E-09	11.5	F315	1 2 0 2 2	
3.040E-12	1.293E-09	17.0	F315	1 2 0 2 2	
5.400E-12	2.297E-09	21.0	F315	1 2 0 2 2	
6.030E-12	2.565E-09	26.0	F315	1 2 0 2 2	
1.481E-11	6.300E-09	40	F303	1 2 1 2 1	
1.490E-11	6.337E-09	41.0	F315	1 2 0 2 2	

2566. C₁₂HCl₉

2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl

2,3,4,5,6,2',3',4',5'-Nonachlorobiphenyl

RN: 40186-72-9 MP (°C): 204.5

MW: 464.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-10	7.800E-08	22	O311	2 2 1 2 1	
5.490E-11	2.549E-08	25	D331	2 1 2 2 2	
5.493E-11	2.550E-08	25	D335	1 0 0 0 2	
2.413E-10	1.120E-07	25	W025	1 0 2 2 2	
5.490E-11	2.549E-08	25.0	M324	1 2 1 1 2	
1.100E-10	5.106E-08	32	D331	2 1 2 2 2	
1.100E-10	5.106E-08	32.0	M324	1 2 1 1 2	
1.420E-10	6.592E-08	40	D331	2 1 2 2 2	
1.420E-10	6.592E-08	40.0	M324	1 2 1 1 2	
2.840E-10	1.318E-07	50	D331	2 1 2 2 2	
2.840E-10	1.318E-07	50.0	M324	1 2 1 1 2	

2567. C₁₂HCl₉

2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl

1,1'-Biphenyl, 2,2',3,3',4,5,5',6,6'-nonachloro-
PCB 208

RN: 52663-77-1 MP (°C): 182

MW: 464.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.880E-11	1.801E-08	25	M342	1 0 1 1 2	

2568. C₁₂H₂Br₈

Octabromobiphenyl

OBPP

Bromkal 80

RN: 27858-07-7 MP (°C): 225.0

MW: 785.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.183E-08	2.500E-05	25	N326	1 0 0 0 1	average

2569. C₁₂H₂Cl₆O

1,2,3,6,7,8-Hexachlorodibenzofuran

1,2,3,6,7,8-HxCDF

F 121

PCDF 121

2,3,4,7,8,9-Hexachlorodibenzofuran

RN: 57117-44-9 **MP (°C):** 233**MW:** 374.87 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.720E-11	1.769E-08	22.5	F314	1 1 0 2 2	

2570. C₁₂H₂Cl₆O

1,2,3,4,7,8-Hexachlorodibenzofuran

1,2,3,4,7,8-HxCDF

F 118

PCDF 118

RN: 70648-26-9 **MP (°C):** 226**MW:** 374.87 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-11	8.247E-09	22.5	F314	1 1 0 2 2	

2571. C₁₂H₂Cl₆O₂1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin

1,2,3,4,7,8-Hexachlorodibenzo[b,e][1,4]dioxin

1,2,3,4,7,8-Hexachlorodibenzo[1,4]dioxin

1,2,3,4,7,8-HxCDD

D 66

PCDD 66

RN: 39227-28-6 **MP (°C):** 273**MW:** 390.87 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.910E-12	2.310E-09	7.0	F315	1 2 0 2 2	
7.980E-12	3.119E-09	11.5	F315	1 2 0 2 2	
1.070E-11	4.182E-09	17.0	F315	1 2 0 2 2	
1.126E-11	4.400E-09	20	F303	1 2 1 2 1	
1.250E-11	4.886E-09	21.0	F315	1 2 0 2 2	
2.020E-11	7.896E-09	26.0	F315	1 2 0 2 2	
4.861E-11	1.900E-08	40	F303	1 2 1 2 2	
4.860E-11	1.900E-08	41.0	F315	1 2 0 2 2	

2572. C₁₂H₂Cl₈

2,2',3,3',4,4',5,5'-Octachlorobiphenyl

2,3,4,5,2',3',4',5'-Octachlorobiphenyl

PCB 194

RN: 35694-08-7 MP (°C): 156

MW: 429.77 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.885E-10	1.240E-07	22	O311	2 2 1 2 2	
6.329E-10	2.720E-07	25	W025	1 0 2 2 2	

2573. C₁₂H₂Cl₈

2,2',3,3',5,5',6,6'-Octachlorobiphenyl

2,3,5,6,2',3',5',6'-Octachlorobiphenyl

RN: 2136-99-4 MP (°C): 161

MW: 429.77 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.650E-10	1.139E-07	20	D331	2 1 2 2 2	
2.650E-10	1.139E-07	20.0	M324	1 2 1 1 2	
3.420E-10	1.470E-07	25	D331	2 1 2 2 2	
3.420E-10	1.470E-07	25	D335	1 0 0 0 2	
9.150E-10	3.932E-07	25	M342	1 0 1 1 2	
4.188E-10	1.800E-07	25	W025	1 0 2 2 1	
3.420E-10	1.470E-07	25.0	M324	1 2 1 1 2	
4.930E-10	2.119E-07	32	D331	2 1 2 2 2	
4.930E-10	2.119E-07	32.0	M324	1 2 1 1 2	
1.780E-09	7.650E-07	50	D331	2 1 2 2 2	
1.780E-09	7.650E-07	50.0	M324	1 2 1 1 2	

2574. C₁₂H₃Cl₅O

2,3,4,7,8-Pentachlorodibenzofuran

2,3,4,7,8-P5CDF

PeCDF, 2,3,4,7,8-

RN: 57117-31-4 MP (°C): 195.5

MW: 340.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.920E-10	2.356E-07	22.5	F314	1 1 0 2 2	

2575. C₁₂H₃Cl₅O₂

1,2,3,4,7-Pentachlorodibenzo-*p*-dioxin
 Dibenz[b,e][1,4]dioxin, 1,2,3,4,7-pentachloro-
 PCDD 50

RN: 39227-61-7 **MP (°C):** 195
MW: 356.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-10	5.061E-08	7.0	F315	1 2 0 2 2	
1.880E-10	6.701E-08	11.5	F315	1 2 0 2 2	
2.440E-10	8.697E-08	17.0	F315	1 2 0 2 2	
3.367E-10	1.200E-07	20	F303	1 2 1 2 1	
3.450E-10	1.230E-07	21.0	F315	1 2 0 2 2	
4.630E-10	1.650E-07	26.0	F315	1 2 0 2 2	
1.291E-09	4.600E-07	40	F303	1 2 1 2 1	
1.280E-09	4.562E-07	41.0	F315	1 2 0 2 2	

2576. C₁₂H₃Cl₇

2,2',3,3',4,4',5-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,4',5-heptachloro-
 PCB 170
 CB 170

RN: 35065-30-6 **MP (°C):** 134.5
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.778E-09	3.470E-06	20	M336	2 0 2 2 2	

2577. C₁₂H₃Cl₇

2,2',3,4',5,5',6-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,4',5,5',6-heptachloro-
 PCB 187

RN: 52663-68-0 **MP (°C):** 104
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-08	4.510E-06	20	M336	2 0 2 2 2	

2578. C₁₂H₃Cl₇

2,2',3,3',5,5',6-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',5,5',6-heptachloro-
 PCB 178

RN: 52663-67-9 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.236E-08	8.840E-06	20	M336	2 0 2 2 2	

2579. C₁₂H₃Cl₇

2,2',3,3',4,6,6'-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,6,6'-heptachloro-
 PCB 176

RN: 52663-65-7 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-08	5.850E-06	20	M336	2 0 2 2 2	

2580. C₁₂H₃Cl₇

2,2',3,3',4,5,6-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,5,6-heptachloro-
 PCB 173

RN: 68194-16-1 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.052E-08	4.160E-06	20	M336	2 0 2 2 2	

2581. C₁₂H₃Cl₇

2,2',3,3',4,5,6'-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,5,6'-heptachloro-
 PCB 174

RN: 38411-25-5 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.328E-08	5.250E-06	20	M336	2 0 2 2 2	

2582. C₁₂H₃Cl₇

2,2',3,4,4',5',6-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,4,4',5',6-heptachloro-
 PCB 183

RN: 52663-69-1 **MP (°C):** 83
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-08	4.900E-06	20	M336	2 0 2 2 2	

2583. C₁₂H₃Cl₇

2,2',3,3',4,5',6-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,5',6-heptachloro-
 PCB 175

RN: 40186-70-7 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.261E-08	8.940E-06	20	M336	2 0 2 2 2	

2584. C₁₂H₃Cl₇

2,2',3,3',4,4',6-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,4',6-heptachloro-
 PCB 171

RN: 52663-71-5 **MP (°C):** 117
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.042E-08	4.120E-06	20	M336	2 0 2 2 2	
5.490E-09	2.170E-06	25	M342	1 0 1 1 2	
5.490E-09	2.170E-06	ns	M308	0 0 1 1 2	

2585. C₁₂H₃Cl₇

2,2',3,3',4',5,6-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,5',6'-heptachloro-
 PCB 177

RN: 52663-70-4 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.219E-08	4.820E-06	20	M336	2 0 2 2 2	

2586. C₁₂H₃Cl₇

2,2',3,3',4,5,5'-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4,5,5'-heptachloro-
 PCB 172

RN: 52663-74-8 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.088E-08	4.300E-06	20	M336	2 0 2 2 2	

2587. C₁₂H₃Cl₇

2,2',3,4,4',5,5'-Heptachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,4,4',5,5'-heptachloro-
 PCB 180

RN: 35065-29-3 **MP (°C):** 112
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.739E-09	3.850E-06	20	M336	2 0 2 2 2	

2588. C₁₂H₃Cl₇

Heptachlorobiphenyl
 1,1'-Biphenyl, heptachloro-
 Heptachlorodiphenyl

RN: 28655-71-2 **MP (°C):**
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.581E-08	6.250E-06	11.5	D085	0 0 0 0 0	mixed isomers

2589. C₁₂H₃Cl₇

2,2',3,4,5,5',6-Heptachlorobiphenyl
 2,3,4,5,6,2',5'-Heptachlorobiphenyl
 PCB 185

RN: 52712-05-7 **MP (°C):** 147
MW: 395.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.381E-08	5.460E-06	20	M336	2 0 2 2 2	<i>sic</i>
1.189E-09	4.700E-07	25	W025	1 0 2 2 1	

2590. C₁₂H₄Br₆

FireMaster FF-1 (hexabromobiphenyl mixture)

RN: **MP (°C):**
MW: 627.62 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-08	1.100E-05	25	H303	1 0 0 0 1	

2591. C₁₂H₄Br₆

2,2',4,4',6,6'-Hexabromobiphenyl

Hexabromobiphenyl

Polybrominated biphenyl

RN: 36355-01-8 MP (°C): 72

MW: 627.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.954E-04	6.247E-01	26.5	G312	0 0 0 0 0	

2592. C₁₂H₄Br₆

Fire Master BP-6 (hexabromophenyl mixture)

RN: 59536-65-1 MP (°C):

MW: 627.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.753E-08	1.100E-05	25	H303	1 0 0 0 1	

2593. C₁₂H₄Br₆O

2,2',4,4',5,5'-Hexabromodiphenylether

RN: MP (°C):

MW: 643.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.723E-11	3.040E-08	10	K431	0 0 0 0 0	
7.831E-11	5.040E-08	25	K431	0 0 0 0 0	
1.896E-10	1.220E-07	35	K431	0 0 0 0 0	

2594. C₁₂H₄Cl₄O

2,3,7,8-Tetrachlorodibenzofuran

2,3,7,8-T4CDF

RN: 51207-31-9 MP (°C): 227

MW: 305.98 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-09	4.192E-07	22.5	F314	1 1 0 2 2	

2595. C₁₂H₄Cl₄O₂1,2,3,4-Tetrachlorodibenzo-*p*-dioxin

1,2,3,4-TCDD

1,2,3,4-Tetrachlorodibenzo[b,e][1,4]dioxin

RN: 30746-58-8 **MP (°C):** 184–186**MW:** 321.98 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E-10	1.130E-07	4.0	D330	2 2 1 2 2	
4.007E-11	1.290E-08	4.3	L321	2 0 2 2 2	
1.065E-09	3.430E-07	5	S352	2 2 0 2 2	
1.401E-09	4.510E-07	15	S352	2 2 0 2 2	
1.500E-09	4.830E-07	17.3	L321	2 0 2 2 2	
1.708E-09	5.500E-07	25	S352	2 2 0 2 1	average of 2
1.957E-09	6.300E-07	25	S352	2 2 0 2 1	
1.460E-09	4.701E-07	25.0	D330	2 2 1 2 2	
3.541E-09	1.140E-06	35	S352	2 2 0 2 2	
3.630E-09	1.169E-06	40.0	D330	2 2 1 2 2	
6.476E-09	2.085E-06	45	S352	2 2 0 2 2	

2596. C₁₂H₄Cl₄O₂2,3,7,8-Tetrachlorodibenzo-*p*-dioxin

TCDD

2,3,7,8-Tetrachlorodibenzodioxin

RN: 1746-01-6 **MP (°C):** 310**MW:** 321.98 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.994E-11	1.930E-08	22	M340	1 2 2 1 2	
6.212E-10	2.000E-07	ns	C098	0 0 0 0 0	
6.212E-10	2.000E-07	ns	K138	0 0 0 0 2	
6.212E-10	2.000E-07	ns	N320	0 0 0 0 0	
2.457E-11	7.910E-09	rt	A323	0 2 2 1 2	

2597. C₁₂H₄Cl₄O₂1,3,6,8-Tetrachlorodibenzo-*p*-dioxin

PCDD 42

1,3,6,8-Tetrachlorodibenzo[1,4]dioxin

RN: 33423-92-6 **MP (°C):** 219**MW:** 321.98 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.939E-10	3.200E-07	20	F303	1 2 1 2 1	
9.939E-10	3.200E-07	20	W319	1 2 1 2 1	
1.211E-09	3.900E-07	40	F303	1 2 1 2 1	
1.211E-09	3.900E-07	40	W319	1 2 1 2 1	
9.845E-10	3.170E-07	ns	W332	0 1 0 2 2	

2598. C₁₂H₄Cl₄O₂1,2,3,7-Tetrachlorodibenzo-*p*-dioxin

PCDD 29

RN: 67028-18-6 **MP (°C):** 175
MW: 321.98 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.560E-10	2.434E-07	7.0	F315	1 2 0 2 2	
8.120E-10	2.614E-07	11.5	F315	1 2 0 2 2	
1.250E-09	4.025E-07	17.0	F315	1 2 0 2 2	
1.336E-09	4.300E-07	20	F303	1 2 1 2 1	
1.490E-09	4.797E-07	21.0	F315	1 2 0 2 2	
2.260E-09	7.277E-07	26.0	F315	1 2 0 2 2	
3.944E-09	1.270E-06	40	F303	1 2 1 2 1	
4.330E-09	1.394E-06	41.0	F315	1 2 0 2 2	

2599. C₁₂H₄Cl₆

2,2',3,4',5,5'-Hexachlorobiphenyl

1,1'-Biphenyl, 2,2',3,4',5,5'-hexachloro-
PCB 146

RN: 51908-16-8 **MP (°C):**
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.103E-08	7.590E-06	20	M336	2 0 2 2 2	

2600. C₁₂H₄Cl₆

2,2',3,3',4,4'-Hexachlorobiphenyl

2,3,4,2',3',4'-Hexachlorobiphenyl

PCB 128

1,1'-Biphenyl, 2,2',3,3',4,4'-hexachloro-
RN: 38380-07-3 **MP (°C):** 150
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.857E-08	6.700E-06	20	M336	2 0 2 2 2	<i>sic</i>
9.690E-10	3.497E-07	25	D306	2 1 2 2 2	
7.840E-10	2.829E-07	25	M342	1 0 1 1 2	
1.219E-09	4.400E-07	25	W025	1 0 2 2 1	

2601. C₁₂H₄Cl₆

2,2',3,3',4,5-Hexachlorobiphenyl

2,3,4,5,2',3'-Hexachlorobiphenyl

2,2',3,3',4,5'-Hexachlorobiphenyl

PCB 129

RN: 55215-18-4 MP (°C): 101

MW: 360.88 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.577E-08	5.690E-06	20	M336	2 0 2 2 2	
1.610E-08	5.810E-06	25	D306	2 1 2 2 2	
2.355E-09	8.500E-07	25	W025	1 0 2 2 1	

2602. C₁₂H₄Cl₆

2,3,3',4,4',5-Hexachlorobiphenyl

2,3,3',4,4',5-Hexachlorobiphenyl

RN: 38380-08-4 MP (°C): 127

MW: 360.88 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.477E-08	5.330E-06	20	M336	2 0 2 2 2	

2603. C₁₂H₄Cl₆

2,2',3,3',6,6'-Hexachlorobiphenyl

1,1'-Biphenyl, 2,2',3,3',6,6'-hexachloro-, (+)-

(+) -PCB 136

RN: 207004-30-6 MP (°C): 114

MW: 360.88 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.050E-09	1.101E-06	4	D331	2 1 2 2 2	
3.050E-09	1.101E-06	4.0	M324	1 2 1 1 2	
9.010E-09	3.252E-06	20	D331	2 1 2 2 2	
5.586E-08	2.016E-05	20	M336	2 0 2 2 2	
9.010E-09	3.252E-06	20.0	M324	1 2 1 1 2	
1.250E-08	4.511E-06	25	D331	2 1 2 2 2	
1.250E-08	4.510E-06	25	D335	1 0 0 0 2	
1.670E-08	6.027E-06	25	M342	1 0 1 1 2	
1.250E-08	4.511E-06	25.0	M324	1 2 1 1 2	
1.850E-08	6.676E-06	32	D331	2 1 2 2 2	
1.850E-08	6.676E-06	32.0	M324	1 2 1 1 2	
1.670E-08	6.027E-06	ns	M308	0 0 1 1 2	

2604. C₁₂H₄Cl₆

2,2',3,3',5,6'-Hexachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',5,6'-hexachloro-
 PCB 135

RN: 52744-13-5 **MP (°C):**
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.586E-08	1.294E-05	20	M336	2 0 2 2 2	

2605. C₁₂H₄Cl₆

2,3,3',4',5,6-Hexachlorobiphenyl
 1,1'-Biphenyl, 2,3,3',4',5,6-hexachloro-
 PCB 163

RN: 74472-44-9 **MP (°C):** 122
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.469E-08	5.300E-06	25	B319	2 0 1 2 1	
1.471E-08	5.310E-06	25	H341	1 0 0 0 2	

2606. C₁₂H₄Cl₆

2,3,3',4,4',6-Hexachlorobiphenyl
 1,1'-Biphenyl, 2,3,3',4,4',6-hexachloro-
 PCB 158

RN: 74472-42-7 **MP (°C):** 107
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.236E-08	8.070E-06	20	M336	2 0 2 2 2	

2607. C₁₂H₄Cl₆

Hexachlorobiphenyl
 1,1'-Biphenyl, hexachloro-

RN: 26601-64-9 **MP (°C):**
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.754E-08	9.940E-06	11.5	D085	0 0 0 0 0	mixed isomers

2608. C₁₂H₄Cl₆

Aroclor 1260

Arochlor 1260

RN: 11096-82-5 **MP (°C):**
MW: 360.88 **BP (°C):** 402.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.879E-08	1.400E-05	4	M336	2 0 2 2 1	
3.990E-08	1.440E-05	20	M336	2 0 2 2 2	
6.927E-08	2.500E-05	20	N326	1 0 0 0 1	

2609. C₁₂H₄Cl₆

2,2',3,5,5',6-Hexachlorobiphenyl

1,1'-Biphenyl, 2,2',3,5,5',6-hexachloro-
PCB 151

RN: 52663-63-5 **MP (°C):** 100
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.755E-08	1.355E-05	20	M336	2 0 2 2 2	

2610. C₁₂H₄Cl₆

2,2',3,3',4,6-Hexachlorobiphenyl

2,2',3,4',5',6'-Hexachlorobiphenyl

PCB 131

RN: 61798-70-7 **MP (°C):**
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.358E-08	1.212E-05	20	M336	2 0 2 2 2	

2611. C₁₂H₄Cl₆

2,2',3,3',5,6-Hexachlorobiphenyl

2,3,5,6,2',3'-Hexachlorobiphenyl

RN: 52704-70-8 **MP (°C):** 132
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.588E-08	1.295E-05	20	M336	2 0 2 2 2	<i>sic</i>
2.522E-09	9.100E-07	25	W025	1 0 2 2 1	

2612. C₁₂H₄Cl₆

2,2',3,4,5,5'-Hexachlorobiphenyl

1,1'-Biphenyl, 2,2',3,4,5,5'-hexachloro-
PCB 141

RN: 52712-04-6 **MP (°C):** 85
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.092E-08	7.550E-06	20	M336	2 0 2 2 2	

2613. C₁₂H₄Cl₆

2,2',3,4,5,6-Hexachlorobiphenyl

1,1'-Biphenyl, 2,2',3,4,5,6-hexachloro-
PCB 144

RN: 68194-14-9 **MP (°C):**
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.586E-08	1.294E-05	20	M336	2 0 2 2 2	

2614. C₁₂H₄Cl₆

2,2',4,4',5,5'-Hexachlorobiphenyl

2,4,5,2',4',5'-PCB

2,4,5,2',4',5'-Hexachlorobiphenyl

PCB 129

PCB 153

RN: 35065-27-1 **MP (°C):** 103
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-08	4.619E-06	4.0	D330	2 2 1 2 2	
2.533E-08	9.140E-06	20	M336	2 0 2 2 2	<i>sic</i>
7.759E-09	2.800E-06	22	C413	2 0 2 2 1	
3.187E-09	1.150E-06	22	O311	2 2 1 2 2	
2.632E-09	9.500E-07	24	C053	0 0 0 0 0	
2.632E-09	9.500E-07	24	F071	1 1 2 1 1	
2.632E-09	9.500E-07	24	M344	1 0 0 0 1	
2.390E-09	8.625E-07	25	D306	2 1 2 2 2	
3.325E-09	1.200E-06	25	W025	1 0 2 2 1	
2.340E-08	8.445E-06	25.0	D330	2 2 1 2 2	
3.540E-08	1.278E-05	40	D330	2 2 1 2 2	
2.641E-09	9.530E-07	ns	H058	0 1 2 1 2	

2615. C₁₂H₄Cl₆

2,2',3,4,4',5'-Hexachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,4,4',5'-hexachloro-
 PCB 138
 CB 138
 K 138

RN: 35065-28-2 **MP (°C):** 80.5
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.020E-08	7.290E-06	20	M336	2 0 2 2 2	

2616. C₁₂H₄Cl₆

2,2',3,4,4',6-Hexachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,4,4',6-hexachloro-
 PCB 139

RN: 56030-56-9 **MP (°C):** 73
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.372E-08	1.217E-05	20	M336	2 0 2 2 2	

2617. C₁₂H₄Cl₆

2,2',3,4,4',5-Hexachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,4,4',5-hexachloro-
 PCB 137

RN: 35694-06-5 **MP (°C):** 77
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.328E-08	8.400E-06	20	M336	2 0 2 2 2	

2618. C₁₂H₄Cl₆

2,2',4,4',6,6'-Hexachlorobiphenyl
 1,1'-Biphenyl, 2,2',4,4',6,6'-hexachloro-
 PCB 155

RN: 33979-03-2 **MP (°C):** 112.5
MW: 360.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-09	1.090E-06	22	O311	2 2 1 2 2	
6.280E-09	2.266E-06	25	D306	2 1 2 2 2	
9.120E-09	3.291E-06	25	L322	1 1 2 2 2	
1.130E-09	4.078E-07	25	M342	1 0 1 1 2	
2.494E-09	9.000E-07	25	W025	1 0 2 2 1	
1.130E-09	4.078E-07	ns	M308	0 0 1 1 2	

2619. C₁₂H₅Br₅

2,2',4,5,5'-Pentabromobiphenyl
1,1'-Biphenyl, 2,2',4,5,5'-pentabromo-
PBB 101

RN: 67888-96-4 **MP (°C):**
MW: 548.72 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-10	1.032E-07	4.0	D330	2 2 1 2 2	
8.060E-10	4.423E-07	25	D330	2 2 1 2 2	
1.790E-09	9.822E-07	40.0	D330	2 2 1 2 2	

2620. C₁₂H₅Br₅O

2,2',4,4',5-Pentabromodiphenyl ether
RN: **MP (°C):**
MW: 564.72 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.108E-09	2.320E-06	10	K431	0 0 0 0 0	
7.738E-09	4.370E-06	25	K431	0 0 0 0 0	
1.186E-08	6.700E-06	35	K431	0 0 0 0 0	

2621. C₁₂H₅Cl₃O₂

1,2,4-Trichlorodibenzo-*p*-dioxin
Dibenzo[b,e][1,4]dioxin, 1,2,4-trichloro-
PCDD 14

RN: 39227-58-2 **MP (°C):** 129
MW: 287.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.617E-09	2.190E-06	5	S352	2 2 0 2 2	
1.659E-08	4.770E-06	15	S352	2 2 0 2 2	
2.925E-08	8.410E-06	25	S352	2 2 0 2 2	
2.925E-08	8.410E-06	25	S352	2 2 0 2 2	
5.801E-08	1.668E-05	35	S352	2 2 0 2 2	
9.815E-08	2.822E-05	45	S352	2 2 0 2 2	

2622. C₁₂H₅Cl₅

2,2',3,4,4'-Pentachlorobiphenyl
1,1'-Biphenyl, 2,2',3,4,4'-pentachloro-
PCB 85

RN: 65510-45-4 **MP (°C):**
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.712E-08	2.191E-05	20	M336	2 0 2 2 2	

2623. C₁₂H₅Cl₅

2,2',3,4',6-Pentachlorobiphenyl

2,2',4,6,6'-Pentachlorobiphenyl

PCB 104

RN: 56558-16-8 **MP (°C):** 85
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.208E-07	3.945E-05	20	M336	2 0 2 2 2	
4.770E-08	1.557E-05	25	D306	2 1 2 2 2	

2624. C₁₂H₅Cl₅

2,2',3,3',6-Pentachlorobiphenyl

1,1'-Biphenyl, 2,2',3,3',6-pentachloro-

PCB 84

RN: 52663-60-2 **MP (°C):**
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.440E-07	4.702E-05	20	M336	2 0 2 2 2	

2625. C₁₂H₅Cl₅

2,2',3,3',5-Pentachlorobiphenyl

1,1'-Biphenyl, 2,2',3,3',5-pentachloro-

PCB 83

RN: 60145-20-2 **MP (°C):**
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.648E-08	2.823E-05	20	M336	2 0 2 2 2	

2626. C₁₂H₅Cl₅

2',3,4,5,5'-Pentachlorobiphenyl

1,1'-Biphenyl, 2,3',4',5,5'-pentachloro-

PCB 124

RN: 70424-70-3 **MP (°C):** 105
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.843E-08	1.581E-05	20	M336	2 0 2 2 2	

2627. C₁₂H₅Cl₅

2,2',3',4,5-Pentachlorobiphenyl

1,1'-Biphenyl, 2,2',3,4',5'-pentachloro-

PCB 87

RN: 41464-51-1 **MP (°C):** 81**MW:** 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.703E-08	2.841E-05	20	M336	2 0 2 2 2	

2628. C₁₂H₅Cl₅

2,2',3,4,5'-Pentachlorobiphenyl

2,3,4,2',5'-Pentachlorobiphenyl

PCB 87

RN: 38380-02-8 **MP (°C):** 112**MW:** 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.009E-08	2.941E-05	20	M336	2 0 2 2 2	
1.379E-08	4.500E-06	25	W025	1 0 2 2 1	

2629. C₁₂H₅Cl₅

2,3,3',4',6-Pentachlorobiphenyl

1,1'-Biphenyl, 2,3,3',4',6-pentachloro-

PCB 110

RN: 38380-03-9 **MP (°C):****MW:** 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.829E-08	2.882E-05	20	M336	2 0 2 2 2	

2630. C₁₂H₅Cl₅

2',3,3',4,5-Pentachlorobiphenyl

1,1'-Biphenyl, 2,3,3',4',5'-pentachloro-

PCB 122

RN: 76842-07-4 **MP (°C):****MW:** 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.933E-08	1.284E-05	20	M336	2 0 2 2 2	

2631. C₁₂H₅Cl₅

2,2',3,3',4-Pentachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,3',4-pentachloro-
 PCB 82

RN: 52663-62-4 **MP (°C):** 119
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.908E-08	2.908E-05	20	M336	2 0 2 2 2	

2632. C₁₂H₅Cl₅

2,2',3,4,5-Pentachlorobiphenyl
 2,3,4,5,2'-Pentachlorobiphenyl
 PCB 86

RN: 55312-69-1 **MP (°C):** 112
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.046E-08	2.300E-05	23	W024	0 0 0 0 0	
1.042E-07	3.400E-05	25	B319	2 0 1 2 1	
1.069E-07	3.490E-05	25	H341	1 0 0 0 2	
3.002E-08	9.800E-06	25	W025	1 0 2 2 2	

2633. C₁₂H₅Cl₅

2,2',3,4,6-Pentachlorobiphenyl
 2,3,4,6,2'-Pentachlorobiphenyl
 PCB 88

RN: 55215-17-3 **MP (°C):** 63
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.676E-08	1.200E-05	25	W025	1 0 2 2 2	

2634. C₁₂H₅Cl₅

2,2',3,5',6-Pentachlorobiphenyl
 1,1'-Biphenyl, 2,2',3,5',6-pentachloro-
 PCB 95

RN: 38379-99-6 **MP (°C):** 94
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.658E-07	5.413E-05	20	M336	2 0 2 2 2	

2635. C₁₂H₅Cl₅

2,2',4,4',5-Pentachlorobiphenyl
 1,1'-Biphenyl, 2,2',4,4',5-pentachloro-
 PCB 99

RN: 38380-01-7 **MP (°C):**
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.798E-08	2.219E-05	20	M336	2 0 2 2 2	

2636. C₁₂H₅Cl₅

2,3',4,4',5-Pentachlorobiphenyl
 1,1'-Biphenyl, 2,3',4,4',5-pentachloro-
 PCB 118
 CB 118

RN: 31508-00-6 **MP (°C):** 109
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.117E-08	1.344E-05	20	M336	2 0 2 2 2	

2637. C₁₂H₅Cl₅

2,3,3',4',5-Pentachlorobiphenyl
 1,1'-Biphenyl, 2,3,3',4',5-pentachloro-
 PCB 107

RN: 70424-68-9 **MP (°C):**
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.546E-08	1.484E-05	20	M336	2 0 2 2 2	

2638. C₁₂H₅Cl₅

2,3,4,4',5-Pentachlorobiphenyl
 1,1'-Biphenyl, 2,3,4,4',5-pentachloro-
 PCB 114

RN: 74472-37-0 **MP (°C):** 98
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.895E-08	1.598E-05	20	M336	2 0 2 2 2	

2639. C₁₂H₅Cl₅

2,3,4,5,6-Pentachlorobiphenyl
 1,1'-Biphenyl, 2,3,4,5,6-pentachloro-
 PCB 116

RN: 18259-05-7 **MP (°C):** 123
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.166E-08	1.360E-05	22	O311	2 2 1 2 2	
1.230E-08	4.015E-06	25	D306	2 1 2 2 2	
1.680E-08	5.484E-06	25	M342	1 0 1 1 2	
2.083E-08	6.800E-06	25	W025	1 0 2 2 1	
1.680E-08	5.484E-06	ns	M308	0 0 1 1 2	

2640. C₁₂H₅Cl₅

2,2',4,5,5'-Pentachlorobiphenyl
 2,4,5,2',5'-PCB
 2,2',4,5,5'-PCB

RN: 37680-73-2 **MP (°C):** 77
MW: 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-08	6.137E-06	4	D331	2 1 2 2 2	
1.880E-08	6.137E-06	4.0	M324	1 2 1 1 2	
3.710E-08	1.211E-05	20	D331	2 1 2 2 2	
8.044E-08	2.626E-05	20	M336	2 0 2 2 2	
3.710E-08	1.211E-05	20.0	M324	1 2 1 1 2	
3.063E-08	1.000E-05	24	C053	0 0 0 0 0	
3.370E-08	1.100E-05	24	C311	0 0 0 0 0	EFG
3.063E-08	1.000E-05	24	F071	1 1 2 1 1	
3.063E-08	1.000E-05	24	M344	1 0 0 0 1	
3.370E-08	1.100E-05	25	C313	0 0 0 0 0	
2.070E-08	6.757E-06	25	D306	2 1 2 2 2	
4.720E-08	1.541E-05	25	D331	2 1 2 2 2	
4.718E-08	1.540E-05	25	D335	1 0 0 0 2	
5.920E-08	1.933E-05	25	M342	1 0 1 1 2	
1.287E-08	4.200E-06	25	W025	1 0 2 2 1	
4.720E-08	1.541E-05	25.0	M324	1 2 1 1 2	
6.830E-08	2.230E-05	32	D331	2 1 2 2 2	
6.830E-08	2.230E-05	32.0	M324	1 2 1 1 2	
3.155E-08	1.030E-05	ns	H058	0 1 2 1 2	
5.820E-08	1.900E-05	ns	M118	0 1 1 1 1	
5.920E-08	1.933E-05	ns	M308	0 0 1 1 2	

2641. C₁₂H₅Cl₅

Pentachlorobiphenyl

2,2',4,4',6-Pentachlorobiphenyl

Kanekrol 500

RN: 25429-29-2 MP (°C):

MW: 326.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.341E-08	2.070E-05	11.5	D085	0 0 0 0 0	
9.496E-08	3.100E-05	22.5	G301	0 0 0 0 0	mixed isomers

2642. C₁₂H₅N₅O₁₁

Pantanitrophenylether

Benzene, 2-(2,4-dinitrophenoxy)-1,3,5-trinitro-

RN: 5950-87-8 MP (°C):

MW: 395.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.771E-04	7.000E-02	27	D067	1 2 0 0 0	
4.302E-04	1.700E-01	50	D067	1 2 0 0 1	
2.404E-03	9.500E-01	100	D067	1 2 0 0 1	

2643. C₁₂H₅N₇O₁₂

Hexanitrodiphenylamine

Benzenamine, 2,4,6-trinitro-N-(2,4,6-trinitrophenyl)-

RN: 131-73-7 MP (°C):

MW: 439.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.366E-04	6.000E-02	17	D070	1 2 0 0 0	
4.325E-04	1.900E-01	50	D070	1 2 0 0 1	
7.738E-04	3.399E-01	100	D070	1 2 0 0 1	

2644. C₁₂H₆Br₄

2,2',5,5'-Tetrabromobiphenyl

Tetrabromobiphenyl

RN: 59080-37-4 MP (°C): 143

MW: 469.82 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.630E-03	4.054E+00	26.5	G312	0 0 0 0 0	

2645. C₁₂H₆Br₄O

2,2',4,4'-Tetrabromodiphenylether

RN: MP (°C):

MW: 485.82 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.661E-08	8.070E-06	10	K431	0 0 0 0 0	
3.026E-08	1.470E-05	25	K431	0 0 0 0 0	
5.105E-09	2.480E-06	35	K431	0 0 0 0 0	

2646. C₁₂H₆Cl₂O₂2,7-Dichlorodibenzo-*p*-dioxin

2,7-DCDD

2,8-Dichlorodibenzodioxin

RN: 33857-26-0 MP (°C): 201

MW: 253.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
4.307E-09	1.090E-06	5	S352	2 2 0 2 2	
7.942E-09	2.010E-06	15	S352	2 2 0 2 2	
1.482E-08	3.750E-06	25	S352	2 2 0 2 2	
1.482E-08	3.750E-06	25	S352	2 2 0 2 2	
2.873E-08	7.270E-06	35	S352	2 2 0 2 2	
5.295E-08	1.340E-05	45	S352	2 2 0 2 2	

2647. C₁₂H₆Cl₂O₂2,8-Dichlorodibenzo-*p*-dioxin

2,8-Dichlorodibenzodioxin

PCDD 12

3,6-Dichloro-9,10-dioxaanthracene

RN: 38964-22-6 MP (°C): 151

MW: 253.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
1.746E-08	4.420E-06	5	S352	2 2 0 2 2	
3.394E-08	8.590E-06	15	S352	2 2 0 2 2	
6.599E-08	1.670E-05	25	S352	2 2 0 2 2	
6.614E-08	1.674E-05	25	S352	2 2 0 2 2	
1.088E-07	2.753E-05	35	S352	2 2 0 2 2	
2.035E-07	5.150E-05	45	S352	2 2 0 2 2	

2648. C₁₂H₆Cl₂O₂2,3-Dichlorodibenzo-*p*-dioxin

2,3-Dichlorodibenzodioxin

PCDD 10

RN: 29446-15-9 **MP (°C):** 160**MW:** 253.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.454E-08	3.680E-06	5	S352	2 2 0 2 2	
2.829E-08	7.160E-06	15	S352	2 2 0 2 2	
5.887E-08	1.490E-05	25	S352	2 2 0 2 2	
5.887E-08	1.490E-05	25	S352	2 2 0 2 2	
1.201E-07	3.040E-05	35	S352	2 2 0 2 2	
2.315E-07	5.860E-05	45	S352	2 2 0 2 2	

2649. C₁₂H₆Cl₃NO₃

Quinonamid

2-(Dichloroacetamido)-3-chloro-1,4-naphthoquinone

HOE 13465OH

Chinonamid

2-[(Dichloroacetyl)amino]-3-chloro-1,4-naphthoquinone

RN: 27541-88-4 **MP (°C):** 212.5**MW:** 318.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.418E-06	3.000E-03	23	M161	1 0 0 0 0	pH 4.6

2650. C₁₂H₆Cl₃NO₃

Chlornitrofen

4-Nitrophenyl 2,4,6-trichlorophenyl ether

1,3,5-Trichloro-2-(4-nitrophenoxy)benzene

1',3',5'-Trichlorophenyl-4-nitrophenyl ether

RN: 1836-77-7 **MP (°C):****MW:** 318.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.398E-06	7.640E-04	22	K137	1 1 2 1 0	

2651. C₁₂H₆Cl₄

2,2',4,5-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,2',4,5-tetrachloro-

PCB 48

RN: 70362-47-9 **MP (°C):** 63.9**MW:** 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-07	2.995E-05	20	M336	2 0 2 2 2	
5.630E-08	1.644E-05	25	M342	1 0 1 1 2	

2652. C₁₂H₆Cl₄

2,3',4,6-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,3',4,6-tetrachloro-

PCB 69

RN: 60233-24-1 **MP (°C):** 46**MW:** 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.004E-08	2.045E-05	20	M336	2 0 2 2 2	

2653. C₁₂H₆Cl₄

Aroclor 1254

Arochlor 1254

RN: 11097-69-1 **MP (°C):****MW:** 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-07	3.900E-05	4	M336	2 0 2 2 1	
8.288E-08	2.420E-05	11.5	D085	0 0 0 0 0	
9.623E-08	2.810E-05	16.50	W033	1 0 2 2 2	
8.459E-08	2.470E-05	16.50	W033	1 0 2 2 2	
1.473E-07	4.300E-05	20	M336	2 0 2 2 1	
1.712E-07	5.000E-05	20	N326	1 0 0 0 1	
~1.92E-07	~5.60E-05	ns	H117	0 2 2 2 0	
1.541E-07	4.500E-05	ns	L106	0 0 2 1 1	
1.370E-07	4.000E-05	ns	M184	0 0 0 0 0	

2654. C₁₂H₆Cl₄

Aroclor 1248

Arochlor 1248

RN: 12672-29-6 **MP (°C):****MW:** 291.99 **BP (°C):** 357.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.425E-07	1.000E-04	20	N326	1 0 0 0 2	

2655. C₁₂H₆Cl₄

3,3',5,5'-Tetrachlorobiphenyl

1,1'-Biphenyl, 3,3',5,5'-tetrachloro-

PCB 80

RN: 33284-52-5 **MP (°C):** 164**MW:** 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.220E-09	1.232E-06	25	D306	2 1 2 2 2	

2656. C₁₂H₆Cl₄

3,3',4,4'-Tetrachlorobiphenyl

3,4,3',4'-Tetrachlorobiphenyl

RN: 32598-13-3 **MP (°C):** 183**MW:** 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-10	1.460E-07	4	D331	2 1 2 2 2	
5.000E-10	1.460E-07	4.0	M324	1 2 1 1 2	
1.490E-09	4.351E-07	20	D331	2 1 2 2 2	
1.490E-09	4.351E-07	20.0	M324	1 2 1 1 2	
6.165E-09	1.800E-06	22	O311	2 2 1 2 1	
1.404E-07	4.100E-05	23	W024	0 0 0 0 0	sic
1.880E-09	5.489E-07	25	D306	2 1 2 2 2	
1.950E-09	5.694E-07	25	D331	2 1 2 2 2	
1.949E-09	5.690E-07	25	D335	1 0 0 0 2	
2.569E-09	7.500E-07	25	W025	1 0 2 2 1	
1.950E-09	5.694E-07	25.0	M324	1 2 1 1 2	
4.040E-09	1.180E-06	32	D331	2 1 2 2 2	
4.040E-09	1.180E-06	32.0	M324	1 2 1 1 2	

2657. C₁₂H₆Cl₄

2,4,4',6-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,4,4',6-tetrachloro-

PCB 75

RN: 32598-12-2 **MP (°C):** 65**MW:** 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-07	9.110E-05	25	D306	2 1 2 2 2	

2658. C₁₂H₆Cl₄

2,4,4',5-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,4,4',5-tetrachloro-
 PCB 74

RN: 32690-93-0 **MP (°C):**
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.049E-07	3.064E-05	20	M336	2 0 2 2 2	

2659. C₁₂H₆Cl₄

2,3,4,5-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,3,4,5-tetrachloro-
 PCB 61

RN: 33284-53-6 **MP (°C):** 92
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.390E-08	9.900E-06	25	B319	2 0 1 2 1	
4.780E-08	1.396E-05	25	D306	2 1 2 2 2	
4.677E-08	1.366E-05	25	L322	1 1 2 2 2	
7.170E-08	2.094E-05	25	M342	1 0 1 1 2	
6.575E-08	1.920E-05	25	W025	1 0 2 2 2	
7.170E-08	2.094E-05	ns	M308	0 0 1 1 2	

2660. C₁₂H₆Cl₄

2,3,4,4'-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,3,4,4'-tetrachloro-
 PCB 60

RN: 33025-41-1 **MP (°C):** 142
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.333E-07	3.893E-05	20	M336	2 0 2 2 2	

2661. C₁₂H₆Cl₄

2,3,4,6-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,3,4,6-tetrachloro-
 PCB 64

RN: 52663-58-8 **MP (°C):**
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.207E-07	9.365E-05	20	M336	2 0 2 2 2	

2662. C₁₂H₆Cl₄

2,3,3',4'-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,3,3',4'-tetrachloro-
 PCB 56

RN: 41464-43-1 **MP (°C):**
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.334E-07	3.894E-05	20	M336	2 0 2 2 2	

2663. C₁₂H₆Cl₄

2,3',4,4'-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,3',4,4'-tetrachloro-
 PCB 66

RN: 32598-10-0 **MP (°C):** 128.0
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-07	3.676E-05	20	M336	2 0 2 2 2	

2664. C₁₂H₆Cl₄

2,3',4',5-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,3',4',5-tetrachloro-
 PCB 70

RN: 32598-11-1 **MP (°C):** 106
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.239E-07	3.618E-05	20	M336	2 0 2 2 2	
2.055E-07	6.000E-05	23	W024	0 0 0 0 0	
7.534E-08	2.200E-05	ns	B301	0 2 1 1 1	

2665. C₁₂H₆Cl₄

2,2',6,6'-Tetrachlorobiphenyl
 1,1'-Biphenyl, 2,2',6,6'-tetrachloro-
 PCB 54

RN: 15968-05-5 **MP (°C):** 198.0
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.247E-09	2.700E-06	22	O311	2 2 1 2 1	
4.070E-08	1.188E-05	25	D306	2 1 2 2 2	

2666. C₁₂H₆Cl₄

2,2',5,5'-Tetrachlorobiphenyl
1,1'-Biphenyl, 2,2',5,5'-tetrachloro-
PCB 52

RN: 35693-99-3 **MP (°C):** 87
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.855E-07	1.126E-04	20	M336	2 0 2 2 2	
5.240E-08	1.530E-05	22	O311	2 2 1 2 2	
1.575E-07	4.600E-05	23	W024	0 0 0 0 0	
5.822E-07	1.700E-04	25	B319	2 0 1 2 2	
3.750E-07	1.095E-04	25	D306	2 1 2 2 2	
1.250E-07	3.650E-05	25	H341	1 0 0 0 2	
1.884E-07	5.500E-05	ns	B301	0 2 1 1 1	
9.076E-08	2.650E-05	ns	H058	0 1 2 1 2	
5.480E-08	1.600E-05	ns	M118	0 1 1 1 1	

2667. C₁₂H₆Cl₄

2,2',4,4'-Tetrachlorobiphenyl
1,1'-Biphenyl, 2,2',4,4'-tetrachloro-
PCB 47

RN: 2437-79-8 **MP (°C):** 42.0
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.260E-07	6.600E-05	22	C413	2 0 2 2 1	
1.853E-07	5.410E-05	22	O311	2 2 1 2 2	
5.993E-07	1.750E-04	23	W024	0 0 0 0 0	
7.534E-07	2.200E-04	25	B351	1 0 0 1 1	

2668. C₁₂H₆Cl₄

2,3,4',5-Tetrachlorobiphenyl
1,1'-Biphenyl, 2,3,4',5-tetrachloro-
PCB 63

RN: 74472-34-7 **MP (°C):**
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.997E-08	2.627E-05	20	M336	2 0 2 2 2	

2669. C₁₂H₆Cl₄

2,2',5,6'-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,2',5,6'-tetrachloro-

PCB 53

RN: 41464-41-9 MP (°C): 103

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.717E-07	1.085E-04	20	M336	2 0 2 2 2	
1.630E-07	4.759E-05	25	D306	2 1 2 2 2	

2670. C₁₂H₆Cl₄

2,2',3,5'-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,2',3,5'-tetrachloro-

PCB 44

RN: 41464-39-5 MP (°C): 47

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.426E-07	1.001E-04	20	M336	2 0 2 2 2	
2.226E-07	6.500E-05	23	W024	0 0 0 0 0	
2.740E-07	8.000E-05	25	B319	2 0 1 2 0	

2671. C₁₂H₆Cl₄

2,2',3,4'-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,2',3,4'-tetrachloro-

PCB 42

RN: 36559-22-5 MP (°C): 68

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.083E-07	6.083E-05	20	M336	2 0 2 2 2	

2672. C₁₂H₆Cl₄

2,2',3,6'-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,2',3,6'-tetrachloro-

PCB 46

RN: 41464-47-5 MP (°C):

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.628E-07	1.059E-04	20	M336	2 0 2 2 2	

2673. C₁₂H₆Cl₄

Tetrachlorobiphenyl

1,1'-Biphenyl, tetrachloro-

Pyralene 1498

RN: 26914-33-0 MP (°C):

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.825E-07	5.330E-05	11.5	D085	0 0 0 0 0	mixed isomers

2674. C₁₂H₆Cl₄

2',3,4,5-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,3',4',5'-tetrachloro-

PCB 76

RN: 70362-48-0 MP (°C): 92.0

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.888E-07	5.513E-05	20	M336	2 0 2 2 2	

2675. C₁₂H₆Cl₄

2,2',3,4-Tetrachlorobiphenyl

1,1'-Biphenyl, 2,2',3,4-tetrachloro-

PCB 41

RN: 52663-59-9 MP (°C):

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.219E-07	6.480E-05	20	M336	2 0 2 2 2	

2676. C₁₂H₆Cl₄

2,2',4,5'-Tetrachlorobiphenyl

2,2',4',5-Tetrachlorobiphenyl

PCB 49

RN: 41464-40-8 MP (°C): 67

MW: 291.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.676E-07	7.814E-05	20	M336	2 0 2 2 2	
5.630E-08	1.644E-05	ns	M308	0 0 1 1 2	

2677. C₁₂H₆Cl₄

2,2',3,3'-Tetrachlorobiphenyl
1,1'-Biphenyl, 2,2',3,3'-tetrachloro-
PCB 40

RN: 38444-93-8 **MP (°C):** 121.0
MW: 291.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.764E-07	8.070E-05	20	M336	2 0 2 2 2	
5.822E-07	1.700E-04	23	W024	0 0 0 0 0	
5.340E-08	1.559E-05	25	D306	2 1 2 2 2	

2678. C₁₂H₆Cl₄O₂S

Tetradifon
2,4,5,4'-Tetrachlorodiphenyl sulfone
Tediom
Aracnol K
Akaritox
Rotetra

RN: 116-29-0 **MP (°C):** 148.5
MW: 356.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.404E-07	5.000E-05	10	V301	1 0 0 0 0	
5.617E-04	2.000E-01	50	M161	1 0 0 0 0	
9.549E-07	3.400E-04	50	V301	1 0 0 0 1	

2679. C₁₂H₇BrClNO₂

Halocrinate
7-Bromo-5-chloro-8-quinoliny 2-propenoate
Halocrinate

RN: 34462-96-9 **MP (°C):** 100.5
MW: 312.56 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-05	6.000E-03	20	M161	1 0 0 0 0	

2680. C₁₂H₇ClO₂1-Chlorodibenz-*p*-dioxin

1-Monochlorodibenzodioxin

PCDD 1

RN: 39227-53-7 MP (°C): 98

MW: 218.64 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.220E-07	1.360E-04	5	S352	2 2 0 2 2	
1.066E-06	2.330E-04	15	S352	2 2 0 2 2	
1.907E-06	4.170E-04	25	S352	2 2 0 2 2	
1.907E-06	4.170E-04	25	S352	2 2 0 2 2	
3.316E-06	7.250E-04	35	S352	2 2 0 2 2	
5.671E-06	1.240E-03	45	S352	2 2 0 2 2	

2681. C₁₂H₇ClO₂2-Chlorodibenz-*p*-dioxin2-Monochlorodibenz-*p*-dioxin

PCDD 2

RN: 39227-54-8 MP (°C): 89

MW: 218.64 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-07	1.334E-04	3.90	D330	2 2 1 2 2	
2.904E-07	6.350E-05	5	S352	2 2 0 2 2	
6.266E-07	1.370E-04	15	S352	2 2 0 2 2	
1.363E-06	2.980E-04	25	S352	2 2 0 2 2	average of 2
1.271E-06	2.780E-04	25	S352	2 2 0 2 2	
1.460E-06	3.192E-04	25.0	D330	2 2 1 2 2	
2.987E-06	6.530E-04	35	S352	2 2 0 2 2	
3.430E-06	7.499E-04	39.0	D330	2 2 1 2 2	
5.072E-06	1.109E-03	45	S352	2 2 0 2 2	

2682. C₁₂H₇Cl₂NO₃

Nitrofen

2,4-Dichlorophenyl-4-nitrophenyl ether

RN: 1836-75-5 MP (°C): 70.5

MW: 284.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.520E-06	1.000E-03	22	M061	1 0 0 0 0	
3.344E-05	9.500E-03	22	M161	1 0 0 0 0	
3.520E-06	1.000E-03	ns	B100	0 0 0 0 0	
2.144E-06	6.090E-04	ns	H322	0 0 0 0 0	

2683. C₁₂H₇Cl₃

2,2',4-Trichlorobiphenyl

1,1'-Biphenyl, 2,2',4-trichloro-

RN: 37680-66-3 MP (°C):

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.006E-06	2.592E-04	20	M336	2 0 2 2 2	

2684. C₁₂H₇Cl₃

2,2',6-Trichlorobiphenyl

1,1'-Biphenyl, 2,2',6-trichloro-

RN: 38444-73-4 MP (°C):

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.741E-06	4.483E-04	20	M336	2 0 2 2 2	

2685. C₁₂H₇Cl₃

2,3',6-Trichlorobiphenyl

1,1'-Biphenyl, 2,3',6-trichloro-

RN: 38444-76-7 MP (°C):

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.498E-07	3.858E-05	20	M336	2 0 2 2 2	

2686. C₁₂H₇Cl₃

2,4,5-Trichlorobiphenyl

1,1'-Biphenyl, 2,4,5-trichloro-

RN: 15862-07-4 MP (°C): 77

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-07	8.500E-05	23	W024	0 0 0 0 0	
5.436E-07	1.400E-04	25	B319	2 0 1 2 1	
5.514E-07	1.420E-04	25	H341	1 0 0 0 2	
6.320E-07	1.628E-04	25	M342	1 0 1 1 2	
3.572E-07	9.200E-05	25	W025	1 0 2 2 1	
6.320E-07	1.628E-04	ns	M308	0 0 1 1 2	

2687. C₁₂H₇Cl₃

2,3,4'-Trichlorobiphenyl

1,1'-Biphenyl, 2,3,4'-trichloro-

RN: 38444-85-8 MP (°C): 69

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-07	1.417E-04	20	M336	2 0 2 2 2	

2688. C₁₂H₇Cl₃

2,3,6-Trichlorobiphenyl

1,1'-Biphenyl, 2,3,6-trichloro-

RN: 55702-45-9 MP (°C): 49

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.126E-07	1.320E-04	20	M336	2 0 2 2 2	

2689. C₁₂H₇Cl₃

2,2',3-Trichlorobiphenyl

1,1'-Biphenyl, 2,2',3-trichloro-

RN: 38444-78-9 MP (°C): 28.1

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-06	2.930E-04	20	M336	2 0 2 2 2	

2690. C₁₂H₇Cl₃

2,2',5-Trichlorobiphenyl

1,1'-Biphenyl, 2,2',5-trichloro-

PCB 18

RN: 37680-65-2 MP (°C): 44

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.160E-06	2.986E-04	20	M336	2 0 2 2 2	
1.980E-06	5.099E-04	25	D306	2 1 2 2 2	
2.485E-06	6.400E-04	25	W025	1 0 2 2 2	
4.271E-07	1.100E-04	ns	B301	0 2 1 1 2	
9.629E-07	2.480E-04	ns	H058	0 1 2 1 2	
6.212E-08	1.600E-05	ns	M118	0 1 1 1 1	

2691. C₁₂H₇Cl₃

3,4,4'-Trichlorobiphenyl

3,4,4'-Trichlorobiphenyl

RN: 38444-90-5 MP (°C): 88

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.791E-07	7.189E-05	20	M336	2 0 2 2 2	
3.106E-07	8.000E-05	23	W024	0 0 0 0 0	
5.902E-08	1.520E-05	25	W025	1 0 2 2 2	

2692. C₁₂H₇Cl₃

2,4',5-Trichlorobiphenyl

2,5,4'-Trichlorobiphenyl

PCB 31

RN: 16606-02-3 MP (°C): 67

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.559E-07	1.432E-04	20	M336	2 0 2 2 2	
3.494E-07	9.000E-05	22	O311	2 2 1 2 1	
4.271E-07	1.100E-04	22.5	G301	0 0 0 0 0	
2.912E-07	7.500E-05	ns	B301	0 2 1 1 1	

2693. C₁₂H₇Cl₃

2,4,6-Trichlorobiphenyl

1,1'-Biphenyl, 2,4,6-trichloro-

RN: 35693-92-6 MP (°C): 62.5

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.120E-07	8.036E-05	4.0	D330	2 2 1 2 2	
9.800E-07	2.524E-04	25	D306	2 1 2 2 2	
9.333E-07	2.404E-04	25	L322	1 1 2 2 2	
8.760E-07	2.256E-04	25	M342	1 0 1 1 2	
7.250E-07	1.867E-04	25.0	D330	2 2 1 2 2	
1.690E-06	4.353E-04	40.0	D330	2 2 1 2 2	
8.760E-07	2.256E-04	ns	M308	0 0 1 1 2	

2694. C₁₂H₇Cl₃

2,4,4'-Trichlorobiphenyl

2,4,4'-PCB

RN: 7012-37-5 **MP (°C):** 57
MW: 257.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.465E-07	1.150E-04	20	C302	1 1 2 2 2	
5.559E-07	1.432E-04	20	M336	2 0 2 2 2	
2.601E-07	6.700E-05	22	O311	2 2 1 2 1	
4.271E-07	1.100E-04	24	C311	0 0 0 0 0	EFG
4.504E-07	1.160E-04	25	C313	0 0 0 0 0	
4.530E-07	1.167E-04	25	D306	2 1 2 2 2	
1.010E-06	2.600E-04	25	W025	1 0 2 2 2	

2695. C₁₂H₇Cl₃

Aroclor 1242

Arochlor 1242

RN: 53469-21-9 **MP (°C):**
MW: 257.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.377E-07	1.900E-04	4	M336	2 0 2 2 2	
5.160E-07	1.329E-04	11.5	D085	0 0 0 0 0	
1.076E-06	2.770E-04	20	M336	2 0 2 2 2	
7.766E-07	2.000E-04	20	N326	1 0 0 0 2	
1.747E-07	4.500E-05	ns	L106	0 0 2 1 1	
7.766E-07	2.000E-04	ns	M184	0 0 0 0 0	

2696. C₁₂H₇Cl₃

2',3,4-Trichlorobiphenyl

1,1'-Biphenyl, 2',3,4-trichloro-

RN: 38444-86-9 **MP (°C):** 60.0
MW: 257.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.147E-07	1.326E-04	20	M336	2 0 2 2 2	
1.165E-07	3.000E-05	23	W024	0 0 0 0 0	

2697. C₁₂H₇Cl₃

2,3',5-Trichlorobiphenyl

1,1'-Biphenyl, 2,3',5-trichloro-

RN: 38444-81-4 MP (°C): 40

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.374E-07	1.384E-04	20	M336	2 0 2 2 2	
9.810E-07	2.527E-04	25	D306	2 1 2 2 2	

2698. C₁₂H₇Cl₃

Trichlorobiphenyl

Apirolio 1431C

Pyranol 1499

Pyralene 3011

RN: 25323-68-6 MP (°C):

MW: 257.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.620E-07	1.190E-04	11.5	D085	0 0 0 0 0	mixed isomers

2699. C₁₂H₇Cl₃O₂

Triclosan

5-Chloro-2-(2,4-dichlorophenoxy)-phenol

RN: 3380-34-5 MP (°C): 55.2

MW: 289.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.454E-05	1.000E-02	20	A067	1 0 0 0 0	
		amb	L434	0 0 0 0 0	
3.467E-05	1.004E-02	ns	R427	0 0 0 0 0	

2700. C₁₂H₇NO₂

1,8-Naphthalimide

1,8-Naphthalenedicarboximide

Naphthalimide

1,8-Naphthalenedicarboxylic acid imide

1H-Benz[de]isoquinoline-1,3(2H)-dione

RN: 81-83-4 MP (°C): 292-300

MW: 197.20 BP (°C): 428.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	5.916E-03	23	B410	2 1 2 2 2	

2701. C₁₂H₇N₃O₂

5-Nitro-1,10-phenanthroline

5-Nitro-*o*-phenanthroline

RN: 4199-88-6 **MP (°C):**
MW: 225.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.210E-04	2.725E-02	25.04	B094	1 2 1 2 2	

2702. C₁₂H₇N₅O₈

2,4,5,6-Tetranitrodiphenylamine

RN: **MP (°C):**
MW: 349.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.348E-04	8.199E-02	13.5	D070	1 2 0 0 1	
2.949E-04	1.030E-01	50	D070	1 2 0 0 2	
5.783E-04	2.020E-01	100	D070	1 2 0 0 2	

2703. C₁₂H₇N₅O₈

2,4,2',4'-Tetranitrodiphenylamine

2,4,2',4-Tetranitro-diphenylamin

RN: 2908-76-1 **MP (°C):**
MW: 349.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.727E-04	2.000E-01	100	F300	1 0 0 0 2	

2704. C₁₂H₈

Acenaphthylene

1,2-Dehydroacenaphthalene

Acenaphthalene

RN: 208-96-8 **MP (°C):** 93.5–94.5
MW: 152.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.582E-05	3.930E-03	25	L332	1 1 1 1 2	

2705. C₁₂H₈Br₂

4,4'-Dibromobiphenyl
p,p'-Dibromobiphenyl

RN: 92-86-4 **MP (°C):** 170
MW: 312.02 **BP (°C):** 357

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.841E-02	5.743E+00	26.5	G312	0 0 0 0 0	

2706. C₁₂H₈Br₂O

4,4'-Dibromodiphenylether
bis-p-Bromophenyl ether
Dibromodiphenyl ether, *p,p'*-

RN: 2050-47-7 **MP (°C):** 59 C
MW: 328.01 **BP (°C):** 357 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.878E-07	9.440E-05	10	K431	0 0 0 0 0	
6.585E-07	2.160E-04	25	K431	0 0 0 0 0	
1.171E-06	3.840E-04	35	K431	0 0 0 0 0	

2707. C₁₂H₈Cl₂

2,5-Dichlorobiphenyl
1,1'-Biphenyl, 2,5-dichloro-

RN: 34883-39-1 **MP (°C):** 23
MW: 223.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.454E-06	1.440E-03	23	W024	0 0 0 0 0	
5.000E-06	1.116E-03	25	D306	2 1 2 2 2	
8.700E-06	1.941E-03	25	M342	1 0 1 1 1	
2.600E-06	5.800E-04	25	W025	1 0 2 2 2	
8.516E-07	1.900E-04	ns	B301	0 2 1 1 2	
2.680E-05	5.979E-03	ns	M308	0 0 1 1 2	

2708. C₁₂H₈Cl₂

2,4-Dichlorobiphenyl
1,1'-Biphenyl, 2,4-dichloro-

RN: 33284-50-3 **MP (°C):** 25.0
MW: 223.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.747E-06	6.129E-04	20	M336	2 0 2 2 2	
3.138E-07	7.000E-05	23	W024	0 0 0 0 0	sic
5.065E-06	1.130E-03	25	B319	2 0 1 2 2	
5.065E-06	1.130E-03	25	B350	1 0 0 0 2	
5.150E-06	1.149E-03	25	D306	2 1 2 2 2	

2709. C₁₂H₈Cl₂

2,4'-Dichlorobiphenyl

2,4'-PCB

RN: 34883-43-7 **MP (°C):** 43
MW: 223.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.855E-06	6.370E-04	20	C302	1 1 2 2 2	
2.413E-06	5.383E-04	20	M336	2 0 2 2 2	
2.241E-06	5.000E-04	24	H100	2 0 2 2 0	
2.779E-06	6.200E-04	25	W025	1 0 2 2 2	
2.855E-06	6.370E-04	ns	H058	0 1 2 1 2	

2710. C₁₂H₈Cl₂

2,3'-Dichlorobiphenyl

1,1'-Biphenyl, 2,3'-dichloro-

RN: 25569-80-6 **MP (°C):**
MW: 223.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.599E-06	5.798E-04	20	M336	2 0 2 2 2	

2711. C₁₂H₈Cl₂

2,6-Dichlorobiphenyl

1,1'-Biphenyl, 2,6-dichloro-

PCB 10

RN: 33146-45-1 **MP (°C):** 35
MW: 223.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.420E-06	5.400E-04	22	O311	2 2 1 2 2	
1.080E-05	2.410E-03	25	D306	2 1 2 2 2	
6.230E-06	1.390E-03	25	M342	1 0 1 1 2	
6.230E-06	1.390E-03	ns	M308	0 0 1 1 2	

2712. C₁₂H₈Cl₂

2,2'-Dichlorobiphenyl

2,2'-PCB

RN: 13029-08-8 **MP (°C):** 61
MW: 223.10 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.214E-06	7.170E-04	20	C302	1 1 2 2 2	
5.038E-06	1.124E-03	20	M336	2 0 2 2 2	
3.541E-06	7.900E-04	22.5	G301	0 0 0 0 0	

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2712. C₁₂H₈Cl₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.275E-06	1.400E-03	23	W024	0 0 0 0 0	
4.034E-06	9.000E-04	24	H100	2 0 2 2 0	
5.410E-06	1.207E-03	25	D306	2 1 2 2 2	
3.541E-06	7.900E-04	25	W025	1 0 2 2 2	

2713. C₁₂H₈Cl₂

3,4-Dichlorobiphenyl

1,1'-Biphenyl, 3,4-dichloro-

RN: 2974-92-7 MP (°C): 49.5
 MW: 223.10 BP (°C): 197.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.550E-08	7.920E-06	25	D306	2 1 2 2 2	
4.074E-07	9.089E-05	ns	R424	0 0 0 0 0	

2714. C₁₂H₈Cl₂

4,4'-Dichlorobiphenyl

4,4'-PCB

Dichlorobiphenyl

RN: 2050-68-2 MP (°C): 149
 MW: 223.10 BP (°C): 317

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.488E-06	3.320E-04	11.5	D085	0 0 0 0 0	mixed isomers
2.779E-07	6.200E-05	20	C053	0 0 0 0 0	
2.779E-07	6.200E-05	20	F071	1 1 1 1 1	
2.779E-07	6.200E-05	20	M344	1 0 0 0 1	
2.689E-07	6.000E-05	24	H100	2 0 2 2 0	
2.376E-07	5.300E-05	25	B319	2 0 1 2 2	average of 2
2.062E-07	4.600E-05	25	B350	1 0 0 0 1	
1.630E-07	3.637E-05	25	D306	2 1 2 2 2	
2.913E-07	6.500E-05	25	H341	1 0 0 0 1	
2.510E-07	5.600E-05	25	W025	1 0 2 2 1	

2715. C₁₂H₈Cl₂

3,3'-Dichlorobiphenyl

1,1'-Biphenyl, 3,3'-dichloro-

RN: 2050-67-1 MP (°C): 29
 MW: 223.10 BP (°C): 323.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-06	3.547E-04	25	D306	2 1 2 2 2	

2716. C₁₂H₈Cl₂O₂S

bis(4-Chlorophenyl) sulfone

4,4'-Dichlorodiphenyl sulfone

1,1'-Sulfonylbis(4-chlorobenzene)

p-Chlorophenyl sulfone

RN: 80-07-9 MP (°C): 149 C

MW: 287.17 BP (°C): 397 C

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.741E-07	5.000E-05	22	J420	0 0 0 0 0	pH 6.5

2717. C₁₂H₈Cl₆

Aldrin

1,2,3,4,10,10-Hexachloro-1,4,4α,5,8,8α-hexahydro-1,4:5,8-dimethanonaphthalene

Aldrite

Seedrin

Aldrosol

HHDN

RN: 309-00-2 MP (°C): 104.3

MW: 364.92 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.877E-07	1.050E-04	15	B083	2 2 1 2 2	particle size 5 μm
7.413E-08	2.705E-05	20	B179	0 0 0 0 0	
4.659E-08	1.700E-05	22.5	G301	0 0 0 0 0	
4.898E-07	1.787E-04	24.99	K436	0 0 0 0 0	
4.933E-07	1.800E-04	25	B083	2 2 1 2 2	particle size 5 μm
5.481E-07	2.000E-04	25	M130	1 0 0 0 0	
4.659E-08	1.700E-05	25	W025	1 0 2 2 2	
7.399E-08	2.700E-05	26.5	P027	1 1 2 2 1	
5.481E-07	2.000E-04	26.70	L095	2 2 1 1 2	
7.399E-08	2.700E-05	27	M161	0 0 0 0 1	
9.591E-07	3.500E-04	35	B083	2 2 1 2 2	particle size 5 μm
1.644E-06	6.000E-04	45	B083	2 2 1 2 2	particle size 5 μm
7.399E-08	2.700E-05	ns	I308	0 0 0 0 0	
3.562E-08	1.300E-05	ns	K138	0 0 0 0 2	
1.096E-07	4.000E-05	ns	M110	0 0 0 0 0	EFG

2718. C₁₂H₈Cl₆O

Endrin

1,2,3,4,10,10-Hexachloro-6,7-epoxy-1,4,4 α ,5,6,7,8,8 α -octahydro-1,4-*endo-endo*-5,8-dimethano-naphthalene

Mendrin

Nendrin

RN: 72-20-8**MP (°C):** 228.0**MW:** 380.91**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.413E-07	1.300E-04	15	B083	2 2 1 2 2	particle size 5 μ m
6.607E-07	2.517E-04	24.99	K436	0 0 0 0 0	
6.563E-07	2.500E-04	25	B083	2 2 1 2 2	particle size 5 μ m
6.826E-07	2.600E-04	25	W025	1 0 2 2 2	
1.103E-06	4.200E-04	35	B083	2 2 1 2 2	particle size 5 μ m
1.641E-06	6.250E-04	45	B083	2 2 1 2 2	particle size 5 μ m
6.301E-08	2.400E-05	ns	K138	0 0 0 0 2	
1.050E-06	4.000E-04	ns	M110	0 0 0 0 0	EFG
<2.63E-07	<1.00E-04	ns	N034	0 0 0 0 0	
6.563E-07	2.500E-04	ns	V414	0 0 0 0 0	

2719. C₁₂H₈Cl₆O

Dieldrin

3,4,5,6,9,9-Hexachloro-1 α ,2,2 α ,3,6,6 α ,7,7 α -octahydro-2,7:3,6-dimethanonaphth[2,3-b]oxirene

Alvit

Quintox

Oxralox

RN: 60-57-1**MP (°C):** 175.5**MW:** 380.91**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-07	7.999E-05	10	B324	0 0 0 0 0	
2.100E-07	8.000E-05	10	B324	0 0 0 0 0	
2.363E-07	9.000E-05	15	B083	2 2 1 2 1	particle size 5 μ m
4.898E-07	1.866E-04	20	B179	0 0 0 0 0	
3.675E-07	1.400E-04	20	B324	0 0 0 0 0	
3.676E-07	1.400E-04	20	B324	0 0 0 0 0	
1.229E-06	4.680E-04	22	K137	1 1 2 1 0	
5.129E-07	1.954E-04	24.99	K436	0 0 0 0 0	
5.119E-07	1.950E-04	25	B083	2 2 1 2 2	particle size 5 μ m
4.883E-07	1.860E-04	25	I308	0 0 0 0 0	
6.563E-07	2.500E-04	25	M130	1 0 0 0 1	
5.251E-07	2.000E-04	25	W025	1 0 2 2 2	
1.313E-07	5.000E-05	26	M061	1 0 0 0 0	
4.883E-07	1.860E-04	26.5	P027	1 1 2 2 2	
5.251E-07	2.000E-04	27	B161	2 1 2 2 0	EFG
4.883E-07	1.860E-04	27	M161	0 0 0 0 2	
5.251E-07	2.000E-04	30	B324	0 0 0 0 0	
5.251E-07	2.000E-04	30	B324	0 0 0 0 0	

(continued)

2719. C₁₂H₈Cl₆O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.050E-06	4.000E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.313E-06	5.000E-04	40	B161	2 1 2 2 0	EFG
1.706E-06	6.500E-04	45	B083	2 2 1 2 2	particle size 5 µm
2.363E-06	9.000E-04	50	B161	2 1 2 2 0	EFG
3.544E-06	1.350E-03	60	B161	2 1 2 2 0	EFG
6.511E-06	2.480E-03	70	B161	2 1 2 2 0	EFG
6.563E-07	2.500E-04	ns	H322	0 0 0 0 0	
5.776E-08	2.200E-05	ns	K138	0 0 0 0 2	
7.876E-07	3.000E-04	ns	M110	0 0 0 0 0	EFG
<2.63E-07	<1.00E-04	ns	N034	0 0 0 0 0	
5.119E-07	1.950E-04	ns	V414	0 0 0 0 0	

2720. C₁₂H₈N₂*p*-Phenanthroline*p*-Phenanthrolin

RN: 230-07-9

MP (°C):

MW: 180.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	1.442E+00	ns	K114	0 0 0 0 0	

2721. C₁₂H₈N₂

Phenazine

Dibenzopyrazine

RN: 92-82-0

MP (°C): 175.5

MW: 180.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	2.523E-02	25	K009	1 2 1 1 0	EFG

2722. C₁₂H₈N₂*o*-Phenanthroline

1,10-Phenanthroline

o-Phenanthrolin

RN: 66-71-7

MP (°C): 115

MW: 180.21

BP (°C): >300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.854E-02	3.340E+00	24.99	B444	0 0 0 0 0	
1.526E-02	2.750E+00	25	M155	1 0 1 1 0	EFG
1.490E-02	2.685E+00	25.04	B094	1 2 1 2 2	
1.850E-02	3.334E+00	31	B094	1 2 1 2 2	

(continued)

2722. C₁₂H₈N₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.090E-02	3.766E+00	35	B094	1 2 1 2 2	
2.550E-02	4.595E+00	40.04	B094	1 2 1 2 2	
2.880E-02	5.190E+00	45.44	B094	1 2 1 2 2	
3.410E-02	6.145E+00	50.04	B094	1 2 1 2 2	

2723. C₁₂H₈N₂*m*-Phenanthroline*m*-Phenanthrolin

RN: 230-46-6 MP (°C):

MW: 180.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	7.208E-01	ns	K114	0 0 0 0 0	

2724. C₁₂H₈N₄O₂

4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-benzoyl-1,5-dihydro-

RN: 96448-63-4 MP (°C):

MW: 240.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.828E-05	1.400E-02	22	B428	1 2 1 2 1	

2725. C₁₂H₈N₄O₆

Picrylaniline

2,4,6-Trinitrodiphenylamine

RN: 2919-12-2 MP (°C):

MW: 304.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.888E-05	1.791E-02	25	B335	1 2 0 0 1	

2726. C₁₂H₈O

Dibenzofuran

Diphenylene oxide

DBF

RN: 132-64-9 MP (°C): 83

MW: 168.20 BP (°C): 154

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.820E-06	1.652E-03	4.0	D330	2 2 1 2 2	
5.960E-05	1.002E-02	25	B173	2 0 2 2 2	

(continued)

2726. C₁₂H₈O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-05	3.112E-03	25	L301	1 1 2 2 2	
2.592E-05	4.360E-03	25	O406	0 0 0 0 0	
2.812E-05	4.730E-03	25	O406	0 0 0 0 0	
2.510E-05	4.222E-03	25.0	D330	2 2 1 2 2	
4.140E-05	6.963E-03	39.8	D330	2 2 1 2 2	

2727. C₁₂H₈O₂Dibenzo-*p*-dioxin

Dibenzo[1,4]dioxin

Oxanthrene

Phenodioxin

RN: 262-12-4 **MP (°C):** 119**MW:** 184.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-06	2.118E-04	4.10	D330	2 2 1 2 2	
1.113E-06	2.050E-04	5	S352	2 2 0 2 2	
2.497E-06	4.600E-04	15	S352	2 2 0 2 2	
7.601E-06	1.400E-03	25	O406	0 0 0 0 0	
6.841E-06	1.260E-03	25	O406	0 0 0 0 0	
4.729E-06	8.710E-04	25	S352	2 2 0 2 2	average of 2
4.571E-06	8.420E-04	25	S352	2 2 0 2 2	
4.890E-06	9.007E-04	25.0	D330	2 2 1 2 2	
9.566E-06	1.762E-03	35	S352	2 2 0 2 2	
1.300E-05	2.395E-03	40.0	D330	2 2 1 2 2	
1.771E-05	3.262E-03	45	S352	2 2 0 2 2	

2728. C₁₂H₈O₄

Methoxsalen

Ammoidin

8-Methoxy-2',3',6,7-furocoumarin

Methoxalen

8-Methoxyfuranocoumarin

Oxypsoralen

RN: 298-81-7 **MP (°C):** 148**MW:** 216.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-04	4.756E-02	30	E012	1 2 1 1 0	

2729. C₁₂H₈S

Dibenzothiophene

Diphenylene sulfide

RN: 132-65-0

MP (°C): 97

MW: 184.26

BP (°C): 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.978E-06	1.470E-03	24	H106	1 0 2 2 2	
7.978E-06	1.470E-03	24	M303	1 0 1 1 2	
2.871E-06	5.291E-04	25	L301	1 1 2 2 2	
7.978E-06	1.470E-03	ns	H107	0 0 0 0 2	

2730. C₁₂H₉Br

4-Bromobiphenyl

1,1'-Biphenyl, 4-bromo-

Bromodiphenyl

RN: 92-66-0

MP (°C): 91.5

MW: 233.11

BP (°C): 310.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.010E-06	2.354E-04	4.0	D330	2 2 1 2 2	
2.800E-06	6.527E-04	25.0	D330	2 2 1 2 2	
3.740E-06	8.718E-04	40.0	D330	2 2 1 2 2	

2731. C₁₂H₉Cl

2-Chlorobiphenyl

2-PCB

RN: 2051-60-7

MP (°C): 32

MW: 188.66

BP (°C): 274

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.993E-05	3.760E-03	20	C302	1 1 2 2 2	
3.074E-05	5.800E-03	23	W024	0 0 0 0 0	
4.771E-06	9.000E-04	24	H100	2 0 2 2 0	
4.134E-05	7.800E-03	25	B351	1 0 0 1 1	
2.680E-05	5.056E-03	25	M342	1 0 1 1 2	
2.189E-05	4.130E-03	25	W025	1 0 2 2 2	
2.680E-05	5.056E-03	ns	M308	0 0 1 1 2	

2732. C₁₂H₉Cl

4-Chlorobiphenyl

1-Chloro-4-phenyl benzene

4-Monochloro-biphenyl

RN: 2051-62-9 **MP (°C):** 77
MW: 188.66 **BP (°C):** 291

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.202E-06	1.170E-03	23	W024	0 0 0 0 0	
2.120E-06	4.000E-04	24	H100	2 0 2 2 0	
7.103E-06	1.340E-03	25	B319	2 0 1 2 2	average of 2
6.891E-06	1.300E-03	25	B350	1 0 0 0 2	
6.361E-06	1.200E-03	25	B351	1 0 0 1 1	
6.361E-06	1.200E-03	25	H341	1 0 0 0 2	
7.087E-06	1.337E-03	25	L322	1 1 2 2 2	average of 2
7.079E-06	1.336E-03	25	L322	1 1 2 2 2	average of 2
4.771E-06	9.000E-04	25	W025	1 0 2 2 2	

2733. C₁₂H₉Cl

3-Chlorobiphenyl

3-Chlorobiphenyl

RN: 2051-61-8 **MP (°C):** 16
MW: 188.66 **BP (°C):** 285

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.908E-05	3.600E-03	23	W024	0 0 0 0 0	
9.806E-06	1.850E-03	23	W024	0 0 0 0 0	
1.924E-05	3.630E-03	25	B319	2 0 1 2 2	
6.891E-06	1.300E-03	25	W025	1 0 2 2 2	

2734. C₁₂H₉Cl

Aroclor 1221

Arochlor 1221

RN: 11104-28-2 **MP (°C):**
MW: 188.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.06E-06	>2.00E-04	ns	M184	0 0 0 0 0	

2735. C₁₂H₉ClF₃N₃O

Norflurazon

4-Chloro-5-(methylamino)-2-(α,α,α -trifluoro-*m*-tolyl)-3(2H)-pyridazinone

Zorial

RN: 27314-13-2 **MP (°C):** 177**MW:** 303.67 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.220E-05	2.800E-02	23	M161	1 0 0 0 1	
9.220E-05	2.800E-02	24	C105	2 1 2 2 2	
9.220E-05	2.800E-02	25	B310	1 1 0 0 1	

2736. C₁₂H₉ClN₂

4-Chloroazobenzene

Diazene, (4-chlorophenyl)phenyl-, (E)-

RN: 4340-77-6 **MP (°C):** 88**MW:** 216.67 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-06	4.333E-04	25	B333	0 0 0 0 0	

2737. C₁₂H₉ClO

4-Chlorophenyl phenyl ether

1-Chloro-4-phenoxybenzene

p-Chlorodiphenyl oxide**RN:** 7005-72-3 **MP (°C):****MW:** 204.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.612E-05	3.300E-03	25	B131	1 0 0 0 1	

2738. C₁₂H₉Cl₂NO₂S*N*-(2,3-Chlorophenyl)-benzene-sulfonamide**RN:** **MP (°C):****MW:** 302.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.922E-05	5.809E-03	20	P433	0 0 0 0 0	
2.256E-05	6.816E-03	25	P433	0 0 0 0 0	
2.717E-05	8.209E-03	30	P433	0 0 0 0 0	
3.511E-05	1.061E-02	37	P433	0 0 0 0 0	
4.300E-05	1.299E-02	42	P433	0 0 0 0 0	

2739. C₁₂H₉Cl₂NO₃

Vinclozolin

3-(3,5-Dichlorophenyl)-5-ethenyl-5-methyl-2,4-oxazolidinedione

Ornalin

Vinclozalin

Ronilan

RN: 50471-44-8 **MP (°C):** 108
MW: 286.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.495E-03	1.000E+00	20	M161	1 0 0 0 0	
9.120E-06	2.609E-03	ns	R427	0 0 0 0 0	

2740. C₁₂H₉Cl₃NO₂S

Reserptyl

4'-[Chlorophenyl]-3,4-dichlorophenylbenzene-sulphonamide

RN: **MP (°C):** 127-129
MW: 337.63 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.066E-04	3.600E-02	25	L014	1 0 1 1 1	

2741. C₁₂H₉FN₂O₄

1-Benzoyloxycarbonyl-5-fluorouracil

1(2H)-Pyrimidinecarboxylic acid, 5-fluoro-3,4-dihydro-2,4-dioxo-, phenylmethyl ester

RN: 66999-98-2 **MP (°C):**
MW: 264.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-04	8.000E-02	22	B332	1 1 0 0 1	pH 4.0

2742. C₁₂H₉N

Carbazole

9-Azafluorene

Dibenzo[b,d]pyrrole

Diphenylenimine

9H-Carbazole

Dibenzopyrrole

RN: 86-74-8 **MP (°C):** 245
MW: 167.21 **BP (°C):** 355

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.177E-06	1.200E-03	20	H300	1 1 2 2 1	
5.427E-06	9.075E-04	25	L301	1 1 2 2 2	

2743. C₁₂H₉NO₃

Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1-methyl-

RN: 74103-11-0 MP (°C):

MW: 215.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.253E-07	7.000E-05	25	P089	0 0 0 0 0	
4.321E-07	9.300E-05	37	P089	0 0 0 0 0	
5.529E-07	1.190E-04	51	P089	0 0 0 0 0	

2744. C₁₂H₉NS

Phenothiazine

Dibenzo-1,4-thiazine

Thiodiphenylamine

RN: 92-84-2 MP (°C): 185.1

MW: 199.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.196E-03	20	M177	2 2 2 2 0	EFG
8.000E-06	1.594E-03	25	M177	2 2 2 2 0	EFG
1.000E-05	1.993E-03	30	M177	2 2 2 2 0	EFG

2745. C₁₂H₉N₃O₂

4-Nitroazobenzene

Diazene, (*p*-nitrophenyl)phenyl-, (E)-

RN: 2491-52-3 MP (°C):

MW: 227.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-06	6.362E-04	25	B333	0 0 0 0 0	

2746. C₁₂H₉N₃O₃

Dis. A. 3

4-[(4-Nitrophenyl)azo]phenol

p-Nitrophenylazophenol*p*-Hydroxy-*p*'-nitroazobenzene

RN: 1435-60-5 MP (°C): 216

MW: 243.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	3.892E-03	25	B333	0 0 0 0 0	

2747. C₁₂H₉N₃O₄

2,4-Dinitrodiphenylamine

2,4-Dinitrodiphenylamin

C.I. Disperse yellow 14

RN: 961-68-2 MP (°C): 160

MW: 259.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.466E-04	3.800E-02	15	D070	1 2 0 0 1	
1.543E-04	4.000E-02	15	F300	1 0 0 0 0	
5.100E-06	1.322E-03	25	B333	0 0 0 0 0	<i>sic</i>
3.240E-04	8.399E-02	50	D070	1 2 0 0 1	
5.516E-04	1.430E-01	100	D070	1 2 0 0 2	

2748. C₁₂H₉N₃O₅

C.I. Disperse yellow 1

C.I. Disperse yellow 1

p-(2,4-Dinitroanilino)

2,4-Dinitro-4'-hydroxydiphenylamine

4-Hydroxy-2',4'-dinitrodiphenylamine

RN: 119-15-3 MP (°C): 194

MW: 275.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-06	2.477E-03	25	B333	0 0 0 0 0	
6.195E-05	1.705E-02	60	P313	0 0 0 0 0	average of 2
1.546E-04	4.255E-02	70	P313	0 0 0 0 0	average of 2
2.954E-04	8.130E-02	80	P313	0 0 0 0 0	average of 2
5.559E-04	1.530E-01	90	P313	0 0 0 0 0	average of 2
1.163E-03	3.200E-01	100	P313	0 0 0 0 0	

2749. C₁₂H₉N₅O₃

1-Nicotinoyloxymethyl allopurinol

3-Pyridinecarboxylic acid, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester

RN: 98846-66-3 MP (°C): 242–243

MW: 271.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.429E-04	9.300E-02	22	B322	0 0 0 0 0	

2750. C₁₂H₁₀

Diphenyl
Biphenyl
Phenylbenzene
1,1'-Biphenyl
Lemonene

RN: 92-52-4 **MP (°C):** 69.1
MW: 154.21 **BP (°C):** 254

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.718E-05	2.650E-03	-7	N053	1 0 0 1 0	EFG
1.973E-05	3.042E-03	4.62	N053	1 0 0 1 0	EFG
2.670E-05	4.118E-03	10	J302	2 1 2 2 2	
2.372E-05	3.658E-03	10.13	N053	1 0 0 1 0	EFG
2.918E-05	4.500E-03	14.20	N053	1 0 0 1 0	EFG
3.800E-05	5.860E-03	20	H306	1 0 1 2 1	
4.182E-05	6.450E-03	20	T301	1 2 2 2 2	
3.590E-05	5.536E-03	20.10	N053	1 0 0 1 0	EFG
4.100E-05	6.323E-03	21	A057	2 1 2 2 1	
4.533E-05	6.990E-03	22	C413	2 0 2 2 1	
4.850E-05	7.480E-03	22.5	G301	0 0 0 0 0	
1.187E-04	1.830E-02	23.5	S171	2 1 2 2 2	
2.983E-05	4.600E-03	24	H100	2 0 2 2 1	
5.512E-05	8.500E-03	24	H116	2 1 0 0 2	
4.708E-05	7.260E-03	24.60	W003	2 2 2 2 2	average of 3
3.852E-05	5.940E-03	25	A001	1 0 2 2 2	
4.570E-05	7.048E-03	25	A325	2 1 2 2 2	
4.850E-05	7.480E-03	25	B003	2 2 2 2 2	
3.910E-05	6.030E-03	25	B173	2 0 2 2 2	
4.799E-05	7.400E-03	25	B319	2 0 1 2 1	average of 2
4.409E-05	6.800E-03	25	B351	1 0 0 1 1	
4.831E-05	7.450E-03	25	E004	2 1 2 2 2	
4.850E-05	7.479E-03	25	J302	2 1 2 2 2	
4.863E-05	7.500E-03	25	M040	1 0 0 1 1	
4.539E-05	7.000E-03	25	M064	1 1 2 2 1	
4.850E-05	7.480E-03	25	M130	1 0 0 0 2	
4.350E-05	6.708E-03	25	M342	1 0 1 1 2	
4.540E-05	7.001E-03	25	M342	1 0 1 1 2	
4.234E-04	6.530E-02	25	S005	2 2 2 2 2	
4.910E-05	7.572E-03	25.04	V013	2 2 2 2 2	
4.416E-05	6.811E-03	25.35	N053	1 0 0 1 0	EFG
5.689E-05	8.774E-03	28.95	N053	1 0 0 1 0	EFG
5.700E-05	8.790E-03	29.90	W003	2 2 2 2 2	average of 3
5.525E-05	8.520E-03	30.30	W003	2 2 2 2 2	average of 3
8.624E-05	1.330E-02	38.40	W003	2 2 2 2 2	average of 3
8.624E-05	1.330E-02	40.10	W003	2 2 2 2 2	average of 3
1.219E-04	1.880E-02	47.50	W003	2 2 2 2 2	average of 3
1.381E-04	2.130E-02	50.10	W003	2 2 2 2 2	average of 3
1.381E-04	2.130E-02	50.20	W003	2 2 2 2 2	average of 2
1.855E-04	2.860E-02	54.70	W003	2 2 2 2 2	average of 3

(continued)

2750. C₁₂H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-04	3.620E-02	59.20	W003	2 2 2 2 2	average of 3
2.620E-04	4.040E-02	60.50	W003	2 2 2 2 2	
2.918E-04	4.500E-02	64.50	W003	2 2 2 2 2	average of 3
4.539E-05	7.000E-03	ns	H123	0 0 0 0 0	
4.350E-05	6.708E-03	ns	M308	0 0 1 1 2	
4.539E-05	7.000E-03	ns	M344	0 0 0 0 1	

2751. C₁₂H₁₀

Acenaphthene

1,2-Dihydroacenaphthene

1,8-Ethylenenaphthalene

peri-Ethylenenaphthalene

RN: 83-32-9

MP (°C): 95

MW: 154.21

BP (°C): 279

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.315E-05	3.570E-03	22.20	W003	2 2 2 2 2	
4.780E-05	7.371E-03	25	B173	2 0 2 2 2	
2.250E-05	3.470E-03	25	E004	2 1 2 2 2	
2.218E-05	3.420E-03	25	L332	1 1 1 1 2	
2.548E-05	3.930E-03	25	M064	1 1 2 2 2	
2.550E-05	3.932E-03	25	M342	1 0 1 1 2	
8.889E-07	1.371E-04	25	R084	2 2 2 2 1	sic
2.330E-05	3.593E-03	25.04	V013	2 2 2 2 2	
3.041E-05	4.690E-03	30.00	W003	2 2 2 2 2	average of 3
3.761E-05	5.800E-03	34.50	W003	2 2 2 2 2	average of 3
4.520E-05	6.970E-03	39.30	W003	2 2 2 2 1	average of 3
6.076E-05	9.370E-03	44.70	W003	2 2 2 2 1	average of 3
8.060E-05	1.243E-02	50.10	W003	2 2 2 2 2	average of 3
1.038E-04	1.600E-02	55.60	W003	2 2 2 2 2	average of 3
1.741E-04	2.685E-02	64.50	W003	2 2 2 2 2	average of 3
1.511E-04	2.330E-02	65.20	W003	2 2 2 2 2	average of 3
2.118E-04	3.267E-02	69.80	W003	2 2 2 2 2	average of 3
2.283E-04	3.520E-02	71.90	W003	2 2 2 2 2	
2.568E-04	3.960E-02	73.40	W003	2 2 2 2 2	average of 2
2.597E-04	4.005E-02	74.70	W003	2 2 2 2 2	average of 2
3.981E-05	6.139E-03	ns	D001	0 0 0 0 2	
2.248E-05	3.467E-03	ns	I332	0 0 0 0 1	
2.000E-05	3.084E-03	ns	L060	0 0 0 0 0	average
2.548E-05	3.930E-03	ns	M344	0 0 0 0 2	
2.344E-05	3.615E-03	ns	R424	0 0 0 0 0	

2752. C₁₂H₁₀ClN

4-Amino-4'-chlorodiphenyl

4-Chloro-4'-aminobiphenyl

p-Amino-*p*'-chlorobiphenyl*p*'-Chloro-*p*-phenylaniline

RN: 135-68-2 MP (°C):

MW: 203.67 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-05	4.684E-03	ns	B305	0 2 0 0 1	

2753. C₁₂H₁₀ClNO₂S

N-(2-Chlorophenyl)-benzene-sulfonamide

RN: MP (°C):

MW: 267.74 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.178E-05	1.119E-02	20	P433	0 0 0 0 0	
4.800E-05	1.285E-02	25	P433	0 0 0 0 0	
5.239E-05	1.403E-02	30	P433	0 0 0 0 0	
5.667E-05	1.517E-02	37	P433	0 0 0 0 0	
6.444E-05	1.725E-02	42	P433	0 0 0 0 0	

2754. C₁₂H₁₀ClNO₂S

N-(4-Chlorophenyl)-benzene-sulfonamide

RN: MP (°C):

MW: 267.74 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.611E-05	2.038E-02	20	P433	0 0 0 0 0	
9.333E-05	2.499E-02	25	P433	0 0 0 0 0	
1.244E-04	3.332E-02	30	P433	0 0 0 0 0	
1.789E-04	4.789E-02	37	P433	0 0 0 0 0	
2.189E-04	5.860E-02	42	P433	0 0 0 0 0	

2755. C₁₂H₁₀Cl₂N₂

3,3'-Dichlorobenzidine

3,3'-Dichloro-4,4'-biphenyldiamine

o,o'-Dichlorobenzidine

4,4'-Diamino-3,3'-dichlorobiphenyl

RN: 91-94-1 MP (°C): 132

MW: 253.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-05	3.114E-03	25	B173	2 0 2 2 2	
<3.95E-06	<1.00E-03	30	M311	1 1 2 2 0	

2756. C₁₂H₁₀N₂

Harmane

1-Methyl-9H-pyrido[3,4-b]indole

Aribine

RN: 486-84-0 MP (°C): 235–238

MW: 182.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.010E+00	1.095E+03	15	B413	1 0 2 2 1	
6.250E+00	1.139E+03	16	B413	1 0 2 2 1	
6.710E+00	1.223E+03	17	B413	1 0 2 2 1	
8.360E+00	1.523E+03	20	B413	1 0 2 2 1	
1.364E+01	2.486E+03	37	B413	1 0 2 2 1	
1.434E+01	2.613E+03	38	B413	1 0 2 2 1	
1.617E+01	2.947E+03	45	B413	1 0 2 2 1	

2757. C₁₂H₁₀N₂O

4-Phenylazophenol

4-Hydroxyazobenzene

p-Hydroxyazobenzene

C.I. Solvent yellow 7

RN: 1689-82-3 MP (°C): 150

MW: 198.23 BP (°C): 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.540E-04	9.000E-02	20	F300	1 0 0 0 1	
1.100E-04	2.180E-02	25	B333	0 0 0 0 0	
1.715E-04	3.400E-02	37	H120	1 1 1 1 1	normal saline
4.036E-03	8.000E-01	100	F300	1 0 0 0 1	

2758. C₁₂H₁₀N₂O

Diphenylnitrosamine

Redax

N-Nitroso-*N*-phenylaniline

RN: 86-30-6 MP (°C): 67

MW: 198.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.770E-04	3.509E-02	25	B173	2 0 2 2 2	

2759. C₁₂H₁₀N₂O₂

2,4-Dihydroxyazobenzene

2,4-Dihydroxy-azobenzol

RN: 2051-85-6 MP (°C): 170

MW: 214.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.336E-04	2.000E-01	20	F300	1 0 0 0 0	

2760. C₁₂H₁₀N₂O₃

3-Hydroxyazobenzene

3-Hydroxy-azobenzol

RN: 40038-46-8 MP (°C):

MW: 230.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.475E-03	8.000E-01	100	F300	1 0 0 0 1	

2761. C₁₂H₁₀N₄O₂

C.I. Disperse orange 3

4'-Nitro-4-aminoazobenzene

4-Amino-4'-nitroazobenzene

4-(4-Nitrophenylazo)aniline

RN: 730-40-5 MP (°C): 211

MW: 242.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-06	2.907E-04	25	B333	0 0 0 0 0	

2762. C₁₂H₁₀N₄O₄

C.I. Disperse yellow 9

2,4-Dinitro-4'-aminodiphenylamine

4-Amino-2',4'-dinitrodiphenylamine

C.I. 10375

RN: 6373-73-5 MP (°C): 188

MW: 274.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.645E-03	25	B333	0 0 0 0 0	

2763. C₁₂H₁₀O*p*-Phenylphenol*p*-Hydroxybiphenyl

RN: 92-69-3

MP (°C): 164.5

MW: 170.21

BP (°C): 306.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-04	5.617E-02	25	E014	2 2 2 1 2	pH 7.2
5.875E-05	1.000E-02	25	L021	1 0 0 0 0	

2764. C₁₂H₁₀O*o*-Phenylphenol

2-Phenylphenol

RN: 90-43-7

MP (°C): 56.5

MW: 170.21

BP (°C): 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.790E-04	1.666E-01	25	L021	1 0 0 0 0	
4.110E-03	6.995E-01	25	M061	0 0 0 0 0	
4.112E-03	7.000E-01	25	M161	1 0 0 0 0	
3.162E-04	5.383E-02	rt	D056	0 1 1 1 0	EFG, pH 6-8, <i>sic</i>

2765. C₁₂H₁₀O

Phenyl ether

Diphenyl ether

RN: 101-84-8

MP (°C): 28

MW: 170.21

BP (°C): 259

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.341E-02	3.984E+00	25	B019	1 0 1 2 0	<i>sic</i>
1.060E-04	1.804E-02	25	B173	2 0 2 2 2	
1.234E-04	2.100E-02	25	F071	1 1 2 1 1	
1.100E-04	1.872E-02	25.04	V013	2 2 2 2 2	

2766. C₁₂H₁₀O₂

1-Naphthaleneacetic acid

NAA

RN: 86-87-3

MP (°C): 134

MW: 186.21

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.040E-03	3.799E-01	17	B200	1 0 0 0 1	
2.255E-03	4.198E-01	20	B200	1 0 0 0 1	
1.179E-02	2.195E+00	20	C092	2 2 0 1 2	
2.228E-03	4.148E-01	25	M061	1 0 0 0 2	average of 2

2767. C₁₂H₁₀O₂

2-Hydroxydiphenyl ether

2-Hydroxy-diphenyl-aether

RN: 2417-10-9 MP (°C):

MW: 186.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.907E-04	1.100E-01	20	F300	1 0 0 0 1	

2768. C₁₂H₁₀O₃

β-Naphthoxyacetic acid

(2-Naphthoxy)acetic acid

Phyomone

BNOA

RN: 120-23-0 MP (°C): 155–157

MW: 202.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.330E-04	8.756E-02	25	D088	0 0 0 0 0	
8.100E-04	1.638E-01	35	D088	0 0 0 0 0	
1.100E-05	2.224E-03	45	D088	0 0 0 0 0	

2769. C₁₂H₁₀O₄

Quinhydrone

Chinhydrone

RN: 106-34-3 MP (°C): 171

MW: 218.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.861E-02	4.061E+00	25	B121	1 2 2 1 2	average of 4

2770. C₁₂H₁₁ClN₂O₅S

Furosemide

Frusemide

RN: 54-31-9 MP (°C): 206

MW: 330.75 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.593E-05	1.850E-02	20	B405	1 1 1 2 2	
1.814E-05	6.000E-03	22.5	C438	0 0 0 0 0	
1.784E-05	5.900E-03	25	A408	2 0 1 2 0	
2.691E-05	8.900E-03	25	B405	1 1 1 2 2	Buffer pH 2.0
7.559E-05	2.500E-02	25	B405	1 1 1 2 2	
1.875E-05	6.200E-03	25	F415	0 0 0 0 0	Average
2.210E-04	7.310E-02	30	E049	2 0 2 2 2	

(continued)

2770. C₁₂H₁₁CIN₂O₅S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.023E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.778E-05	5.882E-03	ns	R427	0 0 0 0 0	

2771. C₁₂H₁₁Cl₂NO

Propyzamide

3,5-Dichloro-N-(1,1-dimethyl-2-propynyl)benzamide

Pronamide

Kerb 50W

RH-315

RN: 23950-58-5 MP (°C): 155.5

MW: 256.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.856E-05	1.500E-02	25	M161	1 0 0 0 1	

2772. C₁₂H₁₁I₃N₂O₄

Iodamide

3-Acetamido-5-acetamidomethyl-2,4,6-triiodobenzoic acid

3-Acetylamino-5-acetylaminomethyl-2,4,6-triiodobenzoic acid

Jodomiron 380

Uromiro

Uromiron

RN: 440-58-4 MP (°C):

MW: 627.95 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.777E-03	3.000E+00	20	F045	1 2 2 2 1	
5.096E-03	3.200E+00	40	F045	1 2 2 2 1	
6.211E-03	3.900E+00	60	F045	1 2 2 2 1	

2773. C₁₂H₁₁N

Diphenylamine

4-Aminobiphenyl

RN: 122-39-4 MP (°C): 53.5

MW: 169.23 BP (°C): 302.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-03	3.079E-01	20	B179	0 0 0 0 0	
3.132E-04	5.300E-02	20	H300	1 2 2 2 1	
3.274E-04	5.540E-02	20	T301	1 2 2 2 2	
2.765E-04	4.680E-02	25	F029	1 0 0 0 2	
3.415E-04	5.780E-02	50	T301	1 2 2 2 2	average of 5
3.557E-04	6.020E-02	80	T301	1 2 2 2 2	average of 5
1.772E-03	2.999E-01	rt	D021	0 0 1 1 0	

2774. C₁₂H₁₁NO₂

Fenfuram

2-Methyl-N-phenyl-3-furancarboxamide

Pano-ram

RN: 24691-80-3 **MP (°C):** 109.5**MW:** 201.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.970E-04	1.000E-01	20	M161	1 0 0 0 0	

2775. C₁₂H₁₁NO₂

Carbaryl

1-Naphthyl N-methylcarbamate

Devicarb

Hexavin

Karbaspary

Murvin

RN: 63-25-2 **MP (°C):** 142**MW:** 201.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-04	5.453E-02	5	H343	0 0 0 0 0	
3.598E-04	7.239E-02	10	B324	0 0 0 0 0	
3.444E-04	6.930E-02	10	B324	0 0 0 0 0	
3.150E-04	6.339E-02	10	H343	0 0 0 0 0	
3.740E-04	7.526E-02	15	H343	0 0 0 0 0	
1.995E-04	4.015E-02	20	B179	0 0 0 0 0	
5.164E-04	1.039E-01	20	B300	2 1 1 1 2	
4.947E-04	9.955E-02	20	B324	0 0 0 0 0	
5.168E-04	1.040E-01	20	B324	0 0 0 0 0	
2.485E-04	5.000E-02	20	F311	1 2 2 2 1	
4.450E-04	8.955E-02	20	H343	0 0 0 0 0	
1.690E-04	3.400E-02	22	K137	1 1 2 1 0	
1.988E-04	4.000E-02	22.5	G301	0 0 0 0 0	
5.210E-04	1.048E-01	25	H343	0 0 0 0 0	
6.184E-04	1.244E-01	30	B324	0 0 0 0 0	
6.460E-04	1.300E-01	30	B324	0 0 0 0 0	
1.988E-04	4.000E-02	30	D089	2 2 0 0 0	
6.520E-04	1.312E-01	30	H343	0 0 0 0 0	
1.988E-04	4.000E-02	30	M161	1 0 0 0 1	
7.860E-04	1.582E-01	35	H343	0 0 0 0 0	
8.990E-04	1.809E-01	40	H343	0 0 0 0 0	
1.006E-03	2.024E-01	45	H343	0 0 0 0 0	
1.988E-04	4.000E-02	ns	H042	0 0 0 0 1	
2.783E-04	5.600E-02	ns	M110	0 0 0 0 0	EFG

2776. C₁₂H₁₁N₃

C.I. Solvent yellow 1

p-Aminoazobenzene

4-Aminoazobenzene

4-Amino-azobenzol

RN: 60-09-3**MP (°C):** 125**MW:** 197.24**BP (°C):** >360

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.591E-04	1.300E-01	18	F300	1 0 0 0 1	
1.500E-04	2.959E-02	25	B333	0 0 0 0 0	
2.484E-04	4.900E-02	37	H120	1 1 1 1 1	
5.510E-04	1.087E-01	60	B198	1 2 1 1 2	
1.041E-03	2.053E-01	71.80	B198	1 2 1 1 2	
1.907E-03	3.761E-01	84.10	B198	1 2 1 1 2	
3.431E-03	6.767E-01	97.40	B198	1 2 1 1 2	

2777. C₁₂H₁₁N₃

Diazoaminobenzene

1,3-Diphenyltriazene

Anilinoazobenzene

N-(Phenylazo)aniline**RN:** 136-35-6**MP (°C):** 98.0**MW:** 197.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-03	4.998E-01	rt	D021	0 0 1 1 0	

2778. C₁₂H₁₁N₃O₃

Orotic acid benzylamide

Orotamide, *N*-benzyl-**RN:** 13156-36-0**MP (°C):** 260–263**MW:** 245.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.600E-02	1.128E+01	-4	N018	0 0 0 0 0	
8.700E-02	2.134E+01	16	N018	0 0 0 0 0	
1.180E-01	2.894E+01	25	N018	0 0 0 0 0	

2779. C₁₂H₁₁O₄P

Diphenyl phosphate

Phosphoric acid, diphenyl ester

RN: 838-85-7 **MP (°C):** 63
MW: 250.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.08E-03	>2.70E-01	24	H116	2 1 0 0 0	

2780. C₁₂H₁₂

1,5-Dimethylnaphthalene

RN: 571-61-9 **MP (°C):** 81
MW: 156.23 **BP (°C):** 265.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.754E-05	2.740E-03	25	E004	2 1 2 2 2	
2.163E-05	3.380E-03	25	M064	1 1 2 2 2	
2.160E-05	3.375E-03	25	M342	1 0 1 1 2	
2.163E-05	3.380E-03	ns	M344	0 0 0 0 2	

2781. C₁₂H₁₂

1-Ethynaphthalene

RN: 1127-76-0 **MP (°C):** -15
MW: 156.23 **BP (°C):** 258

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-05	8.124E-03	10	S076	2 2 2 2 1	
5.200E-05	8.124E-03	14	S076	2 2 2 2 1	
6.400E-05	9.999E-03	20	S076	2 2 2 2 1	
6.849E-05	1.070E-02	25	M064	1 1 2 2 2	
6.850E-05	1.070E-02	25	M342	1 0 1 1 2	
6.400E-05	9.999E-03	25	S076	2 2 2 2 1	
6.849E-05	1.070E-02	ns	M344	0 0 0 0 2	

2782. C₁₂H₁₂

2,3-Dimethylnaphthalene

RN: 581-40-8 **MP (°C):** 103
MW: 156.23 **BP (°C):** 269

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.274E-05	1.990E-03	25	E004	2 1 2 2 2	
1.920E-05	3.000E-03	25	M064	1 1 2 2 1	
1.920E-05	3.000E-03	25	M342	1 0 1 1 2	
1.920E-05	3.000E-03	ns	M344	0 0 0 0 1	

2783. C₁₂H₁₂

1,3-Dimethylnaphthalene

RN: 575-41-7 **MP (°C):** -5
MW: 156.23 **BP (°C):** 263

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.121E-05	8.000E-03	25	M064	1 1 2 2 1	
5.120E-05	7.999E-03	25	M342	1 0 1 1 2	
5.121E-05	8.000E-03	ns	M344	0 0 0 0 1	

2784. C₁₂H₁₂

2,6-Dimethylnaphthalene

RN: 581-42-0 **MP (°C):** 109
MW: 156.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.280E-05	2.000E-03	25	M064	1 1 2 2 1	
1.280E-05	2.000E-03	25	M342	1 0 1 1 2	
1.280E-05	2.000E-03	ns	M344	0 0 0 0 1	

2785. C₁₂H₁₂

2-Ethynaphthalene

RN: 939-27-5 **MP (°C):** -7.4
MW: 156.23 **BP (°C):** 251.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.895E-05	9.210E-03	20	B356	0 0 0 0 0	
5.121E-05	8.000E-03	25	E004	2 1 2 2 2	

2786. C₁₂H₁₂

1,4-Dimethylnaphthalene

RN: 571-58-4 **MP (°C):** 7.6
MW: 156.23 **BP (°C):** 262

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.544E-05	7.100E-03	4	D351	1 2 1 1 2	
4.744E-05	7.412E-03	10	D351	1 2 1 1 2	
6.081E-05	9.500E-03	20	B318	0 0 0 0 0	EFG
6.062E-05	9.470E-03	20	B356	0 0 0 0 0	
6.167E-05	9.634E-03	25	D351	1 2 1 1 2	
7.297E-05	1.140E-02	25	M064	1 1 2 2 2	
7.300E-05	1.140E-02	25	M342	1 0 1 1 1	
7.944E-05	1.241E-02	40	D351	1 2 1 1 2	
7.297E-05	1.140E-02	ns	M344	0 0 0 0 2	

2787. C₁₂H₁₂CINO

2-Chloro-N-(1-methyl-2-propynyl)acetanilide
Basamaize

RN: 35846-47-0 **MP (°C):** 40
MW: 221.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.255E-03	5.000E-01	20	B200	1 0 0 0 0	

2788. C₁₂H₁₂N₂

Benzidine
Benzidin
p-Diaminobiphenyl

RN: 92-87-5 **MP (°C):** 117
MW: 184.24 **BP (°C):** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.953E-03	3.599E-01	24	H106	1 0 2 2 2	
1.954E-03	3.600E-01	24	M303	1 0 1 1 2	pH 5.9
2.712E-03	4.998E-01	25	B019	1 0 1 2 0	
2.822E-03	5.200E-01	25	B068	2 0 1 1 1	
2.700E-04	4.975E-02	25	H091	1 2 2 2 1	<i>sic</i>
1.465E-03	2.699E-01	rt	N015	0 0 2 2 2	

2789. C₁₂H₁₂N₂

m-Benzidine

3-Benzidine

RN: 2050-89-7 **MP (°C):** 117
MW: 184.24 **BP (°C):** 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.970E-02	1.100E+01	100	F300	1 0 0 0 1	

2790. C₁₂H₁₂N₂OS

2,4-Dimethyl-5-carboxanilidothiazole
G-696

RN: 21452-18-6 **MP (°C):** 141
MW: 232.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.056E-02	2.454E+00	25	M061	1 0 0 0 2	

2791. C₁₂H₁₂N₂O₂S

Dapsone

4,4'-Diaminodiphenyl sulphone

RN: 80-08-0 **MP (°C):** 175
MW: 248.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.638E-04	1.400E-01	25	P351	0 0 0 0 0	pH 7.4
6.444E-04	1.600E-01	25	P351	0 0 0 0 0	
1.530E-03	3.800E-01	37	L037	1 2 2 1 1	
4.027E-04	1.000E-01	ns	K444	0 0 0 0 0	

2792. C₁₂H₁₂N₂O₂S

Sulfabenz

Sulfanilid

RN: 127-77-5 **MP (°C):**
MW: 248.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.819E-02	7.000E+00	100	F300	1 0 0 0 0	

2793. C₁₂H₁₂N₂O₃

Nalidixic acid

NegGRAM

1-Ethyl-1,4-dihydro-7-methyl-4-oxo-1,8-naphthyridine-3-carboxylic acid

Nalidic acid

RN: 389-08-2 **MP (°C):** 228
MW: 232.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.306E-04	1.000E-01	23	G098	1 0 0 0 0	
7.079E-01	1.644E+02	37	O307	1 0 1 2 1	pH 2, EFG
4.306E-04	1.000E-01	ns	K444	0 0 0 0 0	

2794. C₁₂H₁₂N₂O₃

Phenobarbital

5-Ethyl-5-phenylbarbituric acid

Phenylethylmalonylurea

RN: 50-06-6 **MP (°C):** 176
MW: 232.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-03	9.243E-01	15	H018	0 0 0 0 0	
3.680E-03	8.546E-01	15	S149	1 2 2 1 2	anhydrate (continued)

2794. C₁₂H₁₂N₂O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.180E-03	7.385E-01	15	S149	1 2 2 1 2	hydrate
4.736E-03	1.100E+00	20	I009	1 2 2 1 1	EFG, 0.005M HCl
3.789E-03	8.800E-01	20	J030	1 2 2 2 1	
4.521E-03	1.050E+00	20	K143	1 2 2 2 2	form II
5.081E-03	1.180E+00	20	K143	1 2 2 2 2	form III
3.143E-03	7.300E-01	20	N023	1 2 2 1 1	hydrate
4.866E-03	1.130E+00	20	N023	1 2 2 1 2	anhydrate
3.920E-03	9.104E-01	20	S149	1 2 2 1 2	hydrate
4.510E-03	1.047E+00	20	S149	1 2 2 1 2	anhydrate
4.731E-03	1.099E+00	25	A023	1 0 0 1 1	
5.167E-03	1.200E+00	25	B011	2 0 0 1 0	
4.994E-03	1.160E+00	25	B065	1 1 1 1 0	
5.590E-03	1.298E+00	25	E011	2 1 1 2 1	
7.737E-03	1.797E+00	25	E011	2 1 1 2 1	pH 7.0
3.078E-02	7.149E+00	25	E011	2 1 1 2 1	pH 8.0
4.731E-03	1.099E+00	25	F009	2 2 2 2 0	EFG
4.600E-03	1.068E+00	25	G003	1 1 1 1 1	pH 4.7
2.734E-03	6.350E-01	25	H005	1 0 1 2 2	
5.161E-03	1.199E+00	25	K010	2 0 0 1 1	
6.114E-03	1.420E+00	25	K143	1 2 2 2 2	form III
5.512E-03	1.280E+00	25	K143	1 2 2 2 2	form II
4.650E-03	1.080E+00	25	L032	2 1 2 0 2	
4.790E-03	1.112E+00	25	M056	2 2 2 2 2	
5.684E-03	1.320E+00	25	N023	1 2 2 1 2	anhydrate
4.995E-03	1.160E+00	25	N023	1 2 2 1 2	hydrate
6.020E-03	1.398E+00	25	P006	2 0 2 2 1	
4.306E-03	1.000E+00	25	P015	0 0 0 0 0	
4.761E-03	1.106E+00	25	P350	0 0 0 0 0	intrinsic
4.830E-03	1.122E+00	25	S149	1 2 2 1 2	hydrate
5.320E-03	1.236E+00	25	S149	1 2 2 1 2	anhydrate
5.170E-03	1.201E+00	25	V033	2 0 1 1 2	
5.200E-03	1.208E+00	25.00	T303	1 0 0 0 1	
6.700E-03	1.556E+00	30	A065	2 0 2 2 1	
6.310E-03	1.465E+00	30	H018	0 0 0 0 0	
6.000E-03	1.393E+00	30	I001	2 0 2 1 0	EFG, 0.003N H ₂ SO ₄
6.100E-03	1.417E+00	30	K108	1 2 2 0 1	
6.502E-03	1.510E+00	30	K143	1 2 2 2 2	form II
7.148E-03	1.660E+00	30	K143	1 2 2 2 2	form III
6.071E-03	1.410E+00	30	N023	1 2 2 1 2	hydrate
6.502E-03	1.510E+00	30	N023	1 2 2 1 2	anhydrate
6.020E-03	1.398E+00	30	O321	0 0 0 0 0	
6.000E-03	1.393E+00	30	O321	0 0 0 0 0	
8.612E-03	2.000E+00	32	M157	2 0 1 1 0	EFG
7.737E-03	1.797E+00	35	A023	1 0 0 1 2	
7.700E-03	1.788E+00	35	S149	1 2 2 1 2	hydrate
7.750E-03	1.800E+00	35	S149	1 2 2 1 2	anhydrate
8.500E-03	1.974E+00	35.00	T303	1 0 0 0 1	

(continued)

2794. C₁₂H₁₂N₂O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.923E-03	1.840E+00	37	J030	1 2 2 2 2	
8.000E-03	1.858E+00	37	K121	1 2 1 2 0	0.1N HCl
9.023E-03	2.096E+00	40	A023	1 0 0 1 2	
9.000E-02	2.090E+01	40	N008	1 0 1 1 2	<i>sic</i>
1.055E-02	2.450E+00	45	S149	1 2 2 1 2	anhydrate
1.108E-02	2.573E+00	45	S149	1 2 2 1 2	hydrate
1.130E-02	2.624E+00	45.00	T303	1 0 0 0 2	
1.266E-02	2.940E+00	50	S149	1 2 2 1 2	anhydrate
1.506E-02	3.498E+00	50	S149	1 2 2 1 2	hydrate
1.698E-02	3.943E+00	55	S149	1 2 2 1 2	hydrate
1.499E-02	3.481E+00	55	S149	1 2 2 1 2	anhydrate
1.033E-02	2.400E+00	60	I009	1 2 2 1 1	EFG, 0.005M HCl
4.306E-03	1.000E+00	ns	K444	0 0 0 0 0	
4.177E-03	9.700E-01	ns	T003	0 0 0 0 2	

2795. C₁₂H₁₂N₂O₆S₂

Benzidine-2,2'-disulfonic acid

Benzidin-disulfosaeure-(2,2')

RN: 117-61-3 MP (°C):

MW: 344.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-03	8.000E-01	25	F300	1 0 0 0 0	

2796. C₁₂H₁₂N₂S

Thiopyrine

1-Phenyl-2,3-dimethyl-3-pyrazoline-5-thione

RN: 5702-69-2 MP (°C): 166

MW: 216.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.600E-02	1.428E+01	ns	D087	0 2 0 0 2	

2797. C₁₂H₁₂N₄O₃

Benznidazole

2-Nitro-N-(phenylmethyl)-imidazole-1-acetamide

RN: 22994-85-0 MP (°C):

MW: 260.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.537E-03	4.000E-01	ns	K444	0 0 0 0 0	

2798. C₁₂H₁₂N₄O₃S

N4-Acetylsulfapyrazine

N4-Acetylsulphapyrazine

RN: 5433-91-0 **MP (°C):**
MW: 292.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	5.000E-02	37	L091	1 0 0 0 0	pH 5.5

2799. C₁₂H₁₂N₄O₃S

N4-Acetyl sulfadiazine

N4-Acetylsulfadiazine

Acetyl sulfadiazine

2-N4-Acetylsulfanilamidopyrimidine

RN: 127-74-2 **MP (°C):**
MW: 292.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
	1.500E-01	37	F075	1 0 2 2 2	
7.200E-04	2.105E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
6.842E-04	2.000E-01	37	L091	1 0 0 0 1	pH 5.5
8.723E-04	2.550E-01	37	M057	1 0 0 0 2	pH 5.5
5.131E-04	1.500E-01	37	R045	1 2 1 1 1	

2800. C₁₂H₁₂N₆O₆

TMPPT

1,3,7,9-Tetramethylpyrimido(5,4-γ) pteridine-2,4,6,8(1H,3H,7H,9H)-tetrone

RN: **MP (°C):**
MW: 336.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.860E-04	1.298E-01	25	K008	1 1 0 1 0	EFG
3.900E-04	1.311E-01	25	K009	1 2 1 1 0	EFG

2801. C₁₂H₁₂O₆

Benzoic acid, 2-(acetoxy)-, (acetoxy)methyl ester

Salicylic acid acetate, hydroxymethyl ester acetate

RN: 32620-68-1 **MP (°C):** oil
MW: 252.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.634E-03	2.430E+00	21	N335	0 0 0 0 0	

2802. C₁₂H₁₃ClN₂O

Buturon

3-(*para*-Chlorophenyl)-1-methyl-1-(1-methyl-2-propynyl) ureaUrea, *N'*-(4-chlorophenyl)-*N*-methyl-*N*-(1-methyl-2-propynyl)

Eptapur

RN: 3766-60-7 MP (°C): 145.5

MW: 236.70 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.267E-04	3.000E-02	20	G036	1 0 0 0 1	
1.267E-04	3.000E-02	20	M161	1 0 0 0 1	

2803. C₁₂H₁₃ClN₄

Pyrimethamine

RN: 58-14-0 MP (°C): 238

MW: 248.72 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.021E-05	1.000E-02	ns	K444	0 0 0 0 0	

2804. C₁₂H₁₃I₃N₂O₂

Iopodic acid

Iopodic acid

RN: 5587-89-3 MP (°C):

MW: 597.96 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.027E-03	1.810E+00	ns	H055	0 0 0 0 0	

2805. C₁₂H₁₃I₃N₂O₃

Iocetamic acid

N-(3-Amino-2,4,6-triiodophenyl)-3-acetamido-2-methylpropionic acid

Cholebrine

MP 620

DRC 1201

RN: 16034-77-8 MP (°C): 224

MW: 613.96 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.610E-03	5.286E+00	37	J016	1 0 0 0 2	pH 7.4

2806. C₁₂H₁₃NO₂

Methsuximide

Celontin

N-Methyl- α -methyl- α -phenylsuccinimide

RN: 77-41-8 MP (°C): 52–53

MW: 203.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.378E-02	2.800E+00	25	P061	0 0 0 0 0	

2807. C₁₂H₁₃NO₂S

Carboxin

2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin

Vitavax

RN: 5234-68-4 MP (°C): 94

MW: 235.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.225E-04	1.700E-01	25	M061	1 0 0 0 2	
7.225E-04	1.700E-01	25	M161	1 0 0 0 2	

2808. C₁₂H₁₃NO₂S

4-Thiazolidinecarboxylic acid, 2-(4-ethenylphenyl)-

RN: 256235-52-6 MP (°C):

MW: 235.31 BP (°C): 464.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-03	8.706E-01	21	B414	1 0 0 1 1	partial decomposition

2809. C₁₂H₁₃NO₃

Azetidine, 1-[(benzoyloxy)acetyl]-

RN: 115178-66-0 MP (°C): 74.5

MW: 219.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.463E-02	5.400E+00	22	N317	1 1 2 1 2	

2810. C₁₂H₁₃NO₃

Crotonyl acetaminophen

Crotonic acid, ester with 4'-hydroxyacetanilide

Acetanilide, 4'-hydroxy-, crotonate (ester)

RN: 20675-24-5 MP (°C): 146-147

MW: 219.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.961E-03	4.300E-01	37	D029	0 0 0 0 0	

2811. C₁₂H₁₃NO₄Acetamide, *N*-acetyl-2-(benzoyloxy)-*N*-methyl-

RN: 115178-80-8 MP (°C):

MW: 235.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-03	3.200E-01	22	N317	1 1 2 1 2	

2812. C₁₂H₁₃NO₄S

Plantvax

2,3-Dihydro-5-carboxanilido-6-methyl-1,4-oxathiin-4,4-dioxide

Oxycarboxin

RN: 5259-88-1 MP (°C): 128.7

MW: 267.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.741E-03	1.000E+00	25	M161	1 0 0 0 0	
3.741E-03	1.000E+00	ns	M061	0 0 0 0 2	

2813. C₁₂H₁₃NO₄S₂

4-Ethylsulfonylnaphthalene-1-sulfonamide

ENS

4-ENS

RN: 842-00-2 MP (°C):

MW: 299.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.775E-04	1.130E-01	c	K042	2 2 2 2 2	

2814. C₁₂H₁₃NO₅

Glycine, *N*-[(benzoyloxy)acetyl]-*N*-methyl-
RN: 106231-64-5 **MP (°C):** 160.5
MW: 251.24 **BP (°C):** 475.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.572E-03	1.400E+00	22	B427	1 0 0 1 1	
5.572E-03	1.400E+00	22	N317	1 1 2 1 2	in 0.01M HCl

2815. C₁₂H₁₃NO₅

Succinyl acetaminophen
 Butanedioic acid, mono[4-(acetylamino)phenyl] ester
 Acetanilide, 4'-hydroxy-, hydrogen succinate ester
RN: 20675-25-6 **MP (°C):** 145.5-146.5
MW: 251.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.587E-02	6.500E+00	37	D029	0 0 0 0 0	

2816. C₁₂H₁₃NO₆

Carbobenzoxypydiglycine
RN: **MP (°C):**
MW: 267.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.432E-03	6.500E-01	25.1	N026	0 0 0 0 0	
2.804E-03	7.494E-01	25.1	N027	1 1 2 2 2	

2817. C₁₂H₁₃N₃O₂

Isocarboxazid
 Marplan
RN: 59-63-2 **MP (°C):**
MW: 231.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.459E-03	8.000E-01	25	R024	0 0 0 0 0	

2818. C₁₂H₁₃N₃O₂S

N1-Methyl-*N*1-2-pyridyl-sulfanilamide
 N1-Methyl-*N*1-(2-pyridyl)sulfanilamide
RN: 51543-29-4 **MP (°C):**
MW: 263.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.740E-03	1.248E+00	37	K095	2 0 0 0 2	intrinsic

2819. C₁₂H₁₃N₃O₃S₂

Methyl acetyl sulfathiazole

Sulfathiazol methyle acetyle

RN: **MP (°C):**
MW: 311.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.248E-04	7.000E-02	37	D084	1 0 1 0 0	

2820. C₁₂H₁₃N₃O₄S

Acetylsulfamethoxazole

Acetanilide, 4'-(5-methyl-3-isoxazolyl)sulfamoyl]-
4'-Acetyl-3-sulfa-5-methylisoxazole

RN: 21312-10-7 **MP (°C):**
MW: 295.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.573E-04	7.600E-02	37	H120	1 1 1 1 1	normal saline

2821. C₁₂H₁₄ClNO₂

Clomazone

Command

Dimethazone

Fenoxan

FMC 57020

Gamit

RN: 81777-89-1 **MP (°C):** 25
MW: 239.70 **BP (°C):** 275.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.592E-03	1.101E+00	ns	S460	0 0 0 0 0	

2822. C₁₂H₁₄Cl₂O₃2,4-Dichlorophenoxyacetic acid *n*-butyl ester

2,4-Dichlorophenoxyacetic acid butyl ester

RN: 94-80-4 **MP (°C):**
MW: 277.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.495E-05	1.523E-02	ns	M120	0 0 1 1 2	

2823. C₁₂H₁₄Cl₂O₃2,4-Dichlorophenoxyacetic acid *sec*-butyl ester

RN: 94-79-1

MP (°C):

MW: 277.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.252E-05	1.733E-02	ns	M120	0 0 1 1 2	

2824. C₁₂H₁₄Cl₃O₄P

Chlorfenvinphos

2-Chloro-1-(2,4-dichlorophenyl)ethenyl phosphoric acid, diethyl ester

Dermatlon

Birlanex

Birlane

Steladone

RN: 470-90-6

MP (°C):

MW: 359.58

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.476E-04	1.250E-01	10	B324	0 0 0 0 0	
3.476E-04	1.250E-01	10	B324	0 0 0 0 0	
4.074E-04	1.465E-01	20	B179	0 0 0 0 0	
3.449E-04	1.240E-01	20	B300	2 1 1 1 2	
3.449E-04	1.240E-01	20	B324	0 0 0 0 0	
3.448E-04	1.240E-01	20	B324	0 0 0 0 0	
3.893E-04	1.400E-01	20	F311	1 2 2 2 1	
4.033E-04	1.450E-01	20	M061	1 0 0 0 2	
4.033E-04	1.450E-01	23	M161	1 0 0 0 2	
2.976E-04	1.070E-01	30	B324	0 0 0 0 0	
2.975E-04	1.070E-01	30	B324	0 0 0 0 0	

2825. C₁₂H₁₄NO₄PS

Ditalimfos

O,O-Diethyl (1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl) phosphonothioate

Laptran

Plondrel

RN: 5131-24-8

MP (°C): 83.5

MW: 299.29

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.444E-04	1.330E-01	rt	M161	0 0 0 0 2	

2826. C₁₂H₁₄N₂O₂

Primidone

5-Ethyldihydro-5-phenyl-4,6(1H,5H)-pyrimidinedione

Desoxyphenobarbitone

2-Deoxyphenobarbital

RN: 125-33-7 MP (°C): 281.5

MW: 218.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.153E-03	4.700E-01	25	C437	0 0 0 0 0	Average
2.200E-03	4.802E-01	30	K108	1 2 2 0 1	
2.747E-03	5.996E-01	37	P061	0 0 0 0 0	
2.291E-03	5.000E-01	rt	D025	0 0 0 0 0	

2827. C₁₂H₁₄N₂O₄

Acetamide, N-(2-amino-2-oxoethyl)-2-(benzoyloxy)-N-methyl-

RN: 106231-62-3 MP (°C): 101.5

MW: 250.26 BP (°C): 496.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E-01	3.020E+01	22	B427	1 0 0 1 1	in 0.01M HCl
1.207E-01	3.020E+01	22	N317	1 1 2 1 2	

2828. C₁₂H₁₄N₂O₄

Propanamide, 2-[[[benzoyloxy)acetyl]amino]-

RN: 115193-30-1 MP (°C): 201.5

MW: 250.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-03	4.800E-01	22	N317	1 1 2 1 2	

2829. C₁₂H₁₄N₂O₅

2-Cyclohexyl-4,6-dinitrophenol

Dinex

4,6-Dinitro-2-cyclohexylphenol

2,4-Dinitro-6-cyclohexylphenol

RN: 131-89-5 MP (°C): 106

MW: 266.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.634E-05	1.500E-02	25	M061	1 0 0 0 1	pH 6.5
6.760E-06	1.800E-03	25	M061	1 0 0 0 1	pH 1

2830. C₁₂H₁₄N₂O₆

Dinoseb acetate

Aretit

RN: 2813-95-8

MP (°C): 26.5

MW: 282.26

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.794E-03	2.200E+00	rt	M161	0 0 0 0 1	

2831. C₁₂H₁₄N₄O₂S

6-Sulfanilamido-2,4-dimethylpyrimidine

6-Sulfanilamido-2,4-dimethylpyrimidin

Sulfisomidine

Sulphasomidine

RN: 515-64-0

MP (°C): 243.0

MW: 278.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.965E-03	1.382E+00	25	M319	2 1 1 1 2	
6.862E-03	1.910E+00	37	K086	1 0 0 0 2	
5.802E-03	1.615E+00	ns	B133	0 2 0 1 2	pH 7.4
1.075E-02	2.991E+00	ns	M141	0 0 0 0 0	

2832. C₁₂H₁₄N₄O₂S

Sulfamethazine

Sulfadimezine

2-Sulfanilamido-4,6,-dimethylpyrimidine

RN: 57-68-1

MP (°C): 176

MW: 278.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.317E-03	1.480E+00	20	F073	1 2 2 2 2	
1.544E-03	4.298E-01	20	L058	1 0 1 1 2	
1.893E-03	5.269E-01	20	O032	1 0 0 0 2	
1.424E-03	3.963E-01	24	N021	2 0 1 2 2	pH 5.6
1.600E-03	4.453E-01	25	M440	0 0 0 0 0	
5.389E-03	1.500E+00	29	C049	0 0 0 0 0	
2.695E-03	7.500E-01	37	L091	1 0 0 0 1	pH 5.5
6.862E-03	1.910E+00	37	M057	1 0 0 0 2	pH 5.5
2.414E-03	6.720E-01	37	S192	1 0 1 1 2	pH 6.0
2.299E-03	6.400E-01	38	K006	1 0 0 0 1	
1.185E-03	3.299E-01	ns	L044	0 0 0 0 2	

2833. C₁₂H₁₄N₄O₂S.0.5H₂O

Sulphamethazine (hemihydrate)

Sulfamethazine hemihydrate

RN: 57-68-1 **MP (°C):**
MW: 287.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.786E-03	1.950E+00	37	R044	0 0 0 0 0	

2834. C₁₂H₁₄N₄O₂S

2-Sulfanilamido-4,5-dimethylpyrimidine

RN: 4462-43-5 **MP (°C):** 225.7
MW: 278.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.186E-04	2.000E-01	29	C049	0 0 0 0 0	

2835. C₁₂H₁₄N₄O₂S

2-Sulfanilyl amino-4-ethylpyrimidine

RN: 2276-96-2 **MP (°C):**
MW: 278.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.180E-04	1.720E-01	37	R076	1 2 0 0 2	

2836. C₁₂H₁₄N₄O₃S₂

Acetyl sulfaethylthiadiazole

Acetamide, N-[4-[[5-(ethyl-1,3,4-thiadiazol-2-yl)amino]sulfonyl]phenyl]-

RN: 1037-51-0 **MP (°C):**
MW: 326.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.963E-03	1.620E+00	37	B046	1 0 2 2 2	pH 4.6

2837. C₁₂H₁₄N₄O₃S

Sulfamethomidine

Sulphamethomidine

RN: 3772-76-7 **MP (°C):** 146.0
MW: 294.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.864E-03	8.430E-01	ns	B133	0 2 0 1 2	pH 7.4
2.884E-03	8.489E-01	ns	R427	0 0 0 0 0	

2838. C₁₂H₁₄N₄O₃S

2-Sulfanilamido-4-ethoxypyrimidine

RN: 71138-72-2 MP (°C):

MW: 294.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.801E-04	5.300E-02	37	R046	1 2 1 1 2	

2839. C₁₂H₁₄N₄O₄S

Sulfadimethoxine

Sulphadimethoxine

RN: 122-11-2 MP (°C): 202.0

MW: 310.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.492E-04	4.630E-02	37	W055	1 2 0 1 2	
1.105E-03	3.430E-01	ns	B133	0 2 0 1 2	pH 7.4

2840. C₁₂H₁₄N₄O₄S

Sulfadoxine

Sulformethoxine

Sulforthomidine

4-Amino-N-(5,6-dimethoxy-4-pyrimidinyl)benzenesulfonamide

Fanzil

Fanasil

RN: 2447-57-6 MP (°C): 190–194

MW: 310.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.761E-04	2.098E-01	ns	R427	0 0 0 0 0	

2841. C₁₂H₁₄O₄

Diethyl phthalate

Ethyl phthalate

Di-ethyl phthalate

Phthalic acid ethyl ester

Phthalsaeure-diaethyl ester

RN: 84-66-2 MP (°C): -40.5

MW: 222.24 BP (°C): 296.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.495E-03	9.990E-01	20	F070	1 0 0 0 0	
4.180E-03	9.290E-01	20	L300	2 1 0 2 2	
1.793E-02	3.984E+00	20.00	D343	0 0 0 0 0	
5.399E-03	1.200E+00	25	F067	1 0 2 2 2	
4.500E-03	1.000E+00	25	F300	1 0 0 0 0	

2842. C₁₂H₁₄O₄

Trimethylacetyl salicylate

Salicylic acid, pivalate

2-Carboxyphenyl pivalate

RN: 2704-58-7 MP (°C):

MW: 222.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.730E-04	2.162E-01	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.74, intrinsic

2843. C₁₂H₁₄O₄Diethyl *o*-phthalate

RN: MP (°C): -40 C

MW: 222.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.618E-03	8.040E-01	25	S417	0 0 0 0 0	

2844. C₁₂H₁₅ClNO₄PS₂

Phosalone

Diethyl *S*-(6-chloro-2-oxobenzoxazolin-3-yl)methyl) phosphorodithioate

Rubitox

Benzophosphate

RN: 2310-17-0 MP (°C):

MW: 367.81 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.263E-06	1.200E-03	10	B324	0 0 0 0 0	
3.263E-06	1.200E-03	10	B324	0 0 0 0 0	
7.069E-06	2.600E-03	20	B300	2 2 1 1 2	
7.069E-06	2.600E-03	20	B324	0 0 0 0 0	
7.069E-06	2.600E-03	20	B324	0 0 0 0 0	
5.845E-06	2.150E-03	20	C053	0 0 0 0 0	
1.006E-05	3.700E-03	30	B324	0 0 0 0 0	
1.006E-05	3.700E-03	30	B324	0 0 0 0 0	
5.845E-06	2.150E-03	ns	F071	0 1 2 1 2	
2.719E-05	1.000E-02	rt	M161	0 0 0 0 1	

2845. C₁₂H₁₅ClO₃

Clofibrate

2-(*p*-Chlorophenoxy)-2-methylpropionic acid ethyl ester

Abitrate

Atromid S

RN: 637-07-0**MP (°C):****MW:** 242.70**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	9.708E-02	rt	G093	0 1 1 1 2	

2846. C₁₂H₁₅IN₂O₆

Uridine, 2'-deoxy-5-iodo-, 5'-propanoate

5'-Propionyl 5-iodo-2'-deoxyuridine

5-Iodo-2'-deoxyuridine 5'-propionate

RN: 84043-25-4 **MP (°C):** 167.5**MW:** 410.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E+03	1.427E+06	25	N332	0 0 0 0 0	pH 7.4

2847. C₁₂H₁₅NO*n*-PropylcinnamamideCinnamamide, *N*-propyl-2-Propenamide, 3-phenyl-*N*-propyl-**RN:** 6329-15-3 **MP (°C):****MW:** 189.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	4.353E-01	ns	H350	0 0 0 0 0	

2848. C₁₂H₁₅NO₃Acetamide, *N*-[2-(benzoyloxy)ethyl]-*N*-methyl-**RN:** 57440-16-1 **MP (°C):****MW:** 221.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-01	3.130E+01	22	N317	1 1 2 1 2	

2849. C₁₂H₁₅NO₃

Acetamide, 2-(benzoyloxy)-*N*-propyl-
RN: 106231-51-0 **MP (°C):** 89.5
MW: 221.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.893E-03	6.400E-01	22	B427	1 0 0 1 1	
2.893E-03	6.400E-01	22	N317	1 1 2 1 2	in 0.01M HCl

2850. C₁₂H₁₅NO₃

Propanamide, 3-(benzoyloxy)-*N,N*-dimethyl-
RN: 115178-77-3 **MP (°C):**
MW: 221.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.955E-02	1.760E+01	22	N317	1 1 2 1 2	

2851. C₁₂H₁₅NO₃

Carbofuran
2,3-Dihydro-2,2-dimethyl-7-benzofuranol methylcarbamate
Crisfuran
Furadanx
Curaterr
RN: 1563-66-2 **MP (°C):** 152
MW: 221.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E-03	2.909E-01	10	B324	0 0 0 0 0	
1.315E-03	2.910E-01	10	B324	0 0 0 0 0	
1.446E-03	3.199E-01	19	B169	2 1 1 1 1	
1.446E-03	3.199E-01	20	B324	0 0 0 0 0	
1.446E-03	3.199E-01	20	B324	0 0 0 0 0	
3.164E-03	7.000E-01	25	M161	1 0 0 0 2	
1.695E-03	3.750E-01	30	B324	0 0 0 0 0	
1.694E-03	3.749E-01	30	B324	0 0 0 0 0	
1.446E-03	3.200E-01	ns	V414	0 0 0 0 0	

2852. C₁₂H₁₅NO₃

Acetaminophen butyrate

Butyryl acetaminophen

Butanoic acid, 4-(acetylamino)phenyl ester

Acetanilide, 4'-hydroxy-, butyrate

RN: 14771-98-3 MP (°C): 140

MW: 221.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.491E-03	3.300E-01	25	B010	1 1 1 1 0	
2.441E-03	5.400E-01	37	D029	0 0 0 0 0	

2853. C₁₂H₁₅NO₃

Acetamide, 2-(benzoyloxy)-N-(1-methylethyl)-

RN: 115193-27-6 MP (°C): 129.5

MW: 221.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.853E-03	4.100E-01	22	N317	1 1 2 1 2	

2854. C₁₂H₁₅NO₄

Isopropyl acetaminophen

Carbonic acid, 4-(acetylamino)phenyl 1-methylethyl ester

Acetanilide, 4'-hydroxy-, isopropyl carbonate

RN: 17239-27-9 MP (°C): 131.5–132

MW: 237.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.636E-03	1.100E+00	37	D029	0 0 0 0 0	

2855. C₁₂H₁₅NO₄

Acetamide, 2-(benzoyloxy)-N-(2-hydroxyethyl)-N-methyl-

RN: 106231-59-8 MP (°C): 79

MW: 237.26 BP (°C): 428.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.135E-02	1.930E+01	22	B427	1 0 0 1 1	in 0.01M HCl
8.135E-02	1.930E+01	22	N317	1 1 2 1 2	

2856. C₁₂H₁₅NO₄*O*-(Butyryloxymethyl) salicylamide*O*-Butyryloxymethyl salicylamide

Butanoic acid, [2-(aminocarbonyl)phenoxy]methyl ester

RN: 103951-39-9 MP (°C): 57

MW: 237.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-02	2.500E+00	23	B328	1 2 2 1 1	pH 4.0
1.054E-02	2.500E+00	23	B328	0 0 0 0 0	

2857. C₁₂H₁₅NO₅

Benzoic acid, 2-hydroxy-, 2-[(2-hydroxyethyl)methylamino]-2-oxoethyl ester

N-Methyl-*N*-carbamoylmethyl glycolamide salicylate

RN: 114665-09-7 MP (°C): 92.5

MW: 253.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.488E-02	6.300E+00	21	B331	1 2 2 1 0	pH 7.4
2.488E-02	6.300E+00	21	B331	0 0 0 0 0	

2858. C₁₂H₁₅NO₆

Ethonyphenyl tartramic acid

RN: MP (°C): 201

MW: 269.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-02	3.989E+00	14	C069	1 2 0 1 2	

2859. C₁₂H₁₅N₂O₃PS

Phoxim

4-Ethoxy-7-phenyl-3,5-dioxa-6-aza-4-phosphaoct-6-ene-8-nitrile 4-sulfide

Baythion

Sebacil

Volation

RN: 14816-18-3 MP (°C):

MW: 298.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.106E-05	3.300E-03	10	B324	0 0 0 0 0	
1.106E-05	3.299E-03	10	B324	0 0 0 0 0	
1.374E-05	4.099E-03	20	B300	2 1 1 1 2	
1.374E-05	4.099E-03	20	B324	0 0 0 0 0	
1.374E-05	4.100E-03	20	B324	0 0 0 0 0	

(continued)

2859. C₁₂H₁₅N₂O₃PS (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.347E-05	7.000E-03	20	M161	1 0 0 0 0	
1.643E-05	4.901E-03	30	B324	0 0 0 0 0	
1.643E-05	4.900E-03	30	B324	0 0 0 0 0	
1.374E-05	4.099E-03	ns	S460	0 0 0 0 0	

2860. C₁₂H₁₅N₂O₃PS

Quinalphos

Diethyl *O*-(2-quinoxalyl) phosphorothioate

Diethquinalphion

Bayrusil

Ekalux

RN: 13593-03-8 MP (°C): 33.5

MW: 298.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.375E-05	2.200E-02	24	M161	1 0 0 0 1	

2861. C₁₂H₁₅N₃O₂S

1-Methyl-2-sulfanilamide-1,2-dihydropyridine

Benzenesulfonamide, 4-amino-*N*-(1,2-dihydro-1-methyl-2-pyridinyl)-

RN: 51543-30-7 MP (°C):

MW: 265.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.690E-03	9.791E-01	37	K095	2 0 0 0 2	intrinsic

2862. C₁₂H₁₅N₃O₂S

Albendazole

Bilutac

Eskazole

Proftril

Valbazan

Zentel

RN: 54965-21-8 MP (°C):

MW: 265.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-06	7.500E-04	209	D426	0 0 0 0 0	
3.769E-05	1.000E-02	ns	K444	0 0 0 0 0	

2863. C₁₂H₁₅N₃O₃

Triallyl cyanurate

Cyanursaeure-triallylaether

RN: 101-37-1 **MP (°C):** 26–28
MW: 249.27 **BP (°C):** 119–120

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.407E-02	6.000E+00	20	F300	1 0 0 0 0	

2864. C₁₂H₁₅N₃O₃S

Albendazole sulphoxide

Ricobendazole

Albendazole oxide

Methoxy-*N*-[5-(propylsulfinyl)benzimidazol-2-yl]carboxamide

Albendazole oxide [BAN:INN]

Carbamic acid

RN: 54029-12-8 **MP (°C):**
MW: 281.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.204E-04	6.200E-02	25	W416	0 0 0 0 0	
1.094E-03	3.079E-01	94.1	D426	0 0 0 0 0	

2865. C₁₂H₁₅N₃O₆1,3,5-Triglycidyl-*S*-triazinetrione

α-TGT

RN: 2451-62-9 **MP (°C):**
MW: 297.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.373E-02	1.300E+01	0	A088	0 0 1 1 1	

2866. C₁₂H₁₅N₅O₅9-[5'-(*O*-Acetyl)-β-D-arabinofuranosyl]adenine ester

Vidarabine 5'-acetate

RN: 65926-28-5 **MP (°C):** 198.0
MW: 309.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.134E-02	6.600E+00	ns	B134	0 1 1 1 1	

2867. C₁₂H₁₅N₅O₅

Pivaloyl salicylate

9-(2-O-Acetyl-β-D-arabinofuranosyl)adenine

RN: 87970-03-4 MP (°C): 195

MW: 309.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.026E-01	9.360E+01	37	B306	1 2 0 1 2	pH 7.3

2868. C₁₂H₁₅O₃P

Diallyl phenyl phosphonate

Phosphonic acid, phenyl-, di-2-propenyl ester

RN: 2948-89-2 MP (°C):

MW: 238.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.259E-03	3.000E-01	25	B070	1 2 0 1 0	

2869. C₁₂H₁₆CINOS

Orbencarb

Lanray

S-((2-Chlorophenyl)methyl) diethylcarbamothioate

RN: 34622-58-7 MP (°C):

MW: 257.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.311E-05	2.400E-02	ns	S460	0 0 0 0 0	

2870. C₁₂H₁₆CINOS

Thiobencarb

S-4-Chlorobenzyl diethylthiocarbamate

Diethylcarbamothioic acid S-[(4-chlorophenyl)methyl] ester

4-Chlorobenzyl N,N-diethylthiocarbamate

RN: 28249-77-6 MP (°C):

MW: 257.78 BP (°C): 127.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.164E-04	3.000E-02	22	K137	1 1 2 1 0	
1.164E-04	3.001E-02	ns	S460	0 0 0 0 0	

2871. C₁₂H₁₆Cl₂N₂O

Neburon

1-Butyl-3-(3,4-dichlorophenyl)-1-methylurea

RN: 555-37-3 MP (°C): 101.5

MW: 275.18 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.744E-05	4.800E-03	20	F311	1 2 2 2 1	
1.744E-05	4.800E-03	24	B185	0 0 0 0 0	
1.744E-05	4.800E-03	24	G036	1 0 0 0 1	
1.744E-05	4.800E-03	24	M061	1 0 0 0 1	
1.744E-05	4.800E-03	24	M161	1 0 0 0 1	
1.744E-05	4.800E-03	25	A039	1 1 0 0 1	
1.744E-05	4.800E-03	25	G099	1 0 0 1 0	
1.744E-05	4.800E-03	ns	K007	0 0 0 0 1	

2872. C₁₂H₁₆N₂

Etryptamine

α-Ethyltryptamine

RN: 2235-90-7 MP (°C): 97

MW: 188.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.709E-03	5.100E-01	rt	M011	0 0 2 1 1	intrinsic

2873. C₁₂H₁₆N₂O

N-(Piperidinomethyl)benzamide

Benzamide, N-(1-pyrrolidinylmethyl)-

RN: 92788-60-8 MP (°C):

MW: 204.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-03	1.450E+00	22	J037	0 0 0 0 0	

2874. C₁₂H₁₆N₂O₂

N,N,N',N'-Tetramethylterephthalamide

1,4-Benzenedicarboxamide, N,N,N',N'-tetramethyl-

RN: 13158-31-1 MP (°C):

MW: 220.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.843E+00	4.060E+02	30	K004	1 0 0 0 2	
1.840E+00	4.053E+02	30	K019	1 0 0 0 2	

2875. C₁₂H₁₆N₂O₂*N,N,N',N'-Tetramethylphthalamide*1,2-Benzenedicarboxamide, *N,N,N',N'-tetramethyl-***RN:** 6329-16-4 **MP (°C):****MW:** 220.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.223E+00	7.100E+02	30	K004	1 0 0 0 2	

2876. C₁₂H₁₆N₂O₂*N,N,N',N'-Tetramethylisophthalamide*1,3-Benzenedicarboxamide, *N,N,N',N'-tetramethyl-***RN:** 14334-36-2 **MP (°C):****MW:** 220.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.069E+00	6.760E+02	30	K004	1 0 0 0 2	
3.070E+00	6.762E+02	30	K019	1 0 0 0 2	

2877. C₁₂H₁₆N₂O₂S

4-Thiazolidinecarboxylic acid, 2-[4-(dimethylamino)phenyl]-

4-Thiazolidinecarboxylic acid, 2-(*p*-dimethylaminophenyl)-**RN:** 72678-86-5 **MP (°C):****MW:** 252.34 **BP (°C):** 481.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-03	6.813E-01	21	B414	1 0 0 1 1	fast decomposition

2878. C₁₂H₁₆N₂O₃*Hexobarbital*

5-(1-Cyclohexen-1-yl)-1,5-dimethylbarbituric acid

5-(1-Cyclohexenyl)-1,5-dimethylbarbituric acid

*Hexabarital***RN:** 56-29-1 **MP (°C):** 146**MW:** 236.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-03	2.900E-01	20	J030	1 2 2 2 1	
1.840E-03	4.347E-01	25	M056	2 2 2 2 2	
2.000E-03	4.725E-01	30	K108	1 2 2 0 1	
2.709E-03	6.400E-01	37	J030	1 2 2 2 1	

2879. C₁₂H₁₆N₂O₃

Carbetamide

N-Ethyl-2-(((phenylamino)carbonyl)oxy)propanamide

Leguarme

RN: 16118-49-3 MP (°C): >110

MW: 236.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.481E-02	3.500E+00	20	M161	1 0 0 0 1	

2880. C₁₂H₁₆N₂O₃

Cyclobarbital

Phanodorm

RN: 52-31-3 MP (°C): 173

MW: 236.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.772E-03	1.600E+00	20	F300	1 0 0 0 1	
6.941E-03	1.640E+00	20	J030	1 2 2 2 2	
3.500E-02	8.270E+00	25	G003	1 1 1 1 1	pH 4.7
8.000E-03	1.890E+00	30	G014	1 1 1 1 0	EFG
7.800E-03	1.843E+00	30	I001	2 0 2 1 0	EFG, 0.003N H ₂ SO ₄
8.000E-03	1.890E+00	30	K108	1 2 2 0 1	
9.735E-03	2.300E+00	37	F300	1 0 0 0 1	
9.523E-03	2.250E+00	37	J030	1 2 2 2 2	
9.140E-02	2.160E+01	40	N008	1 2 1 1 2	sic

2881. C₁₂H₁₆N₃O₃PS

Triazophos

O,O-Diethyl O-(1-phenyl-1H-1,2,4-triazol-3-yl) phosphorothioate

Hostathion

RN: 24017-47-8 MP (°C):

MW: 313.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.884E-05	2.470E-02	20	B300	2 1 1 1 2	
1.245E-04	3.900E-02	23	M161	1 0 0 0 1	
1.245E-04	3.900E-02	23	T305	1 0 0 0 1	
1.245E-04	3.899E-02	ns	S460	0 0 0 0 0	

2882. C₁₂H₁₆N₃O₃PS₂

Azinphos-ethyl

O,O-Diethyl *S*-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate

Azinos

Ethyl guthion

RN: 2642-71-9**MP (°C):****MW:** 345.38**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.940E-05	6.700E-03	10	B324	0 0 0 0 0	
1.940E-05	6.700E-03	10	B324	0 0 0 0 0	
3.040E-05	1.050E-02	20	B300	2 2 1 1 2	
3.040E-05	1.050E-02	20	B324	0 0 0 0 0	
3.040E-05	1.050E-02	20	B324	0 0 0 0 0	
7.152E-05	2.470E-02	30	B324	0 0 0 0 0	
7.151E-05	2.470E-02	30	B324	0 0 0 0 0	
3.020E-05	1.043E-02	ns	R427	0 0 0 0 0	

2883. C₁₂H₁₆N₄O₂

2,5-Diaziridinyl-3,6-bis(methylamino)-1,4-benzoquinone

Benzoquinone-2,5-bisaziridinyl-3,6-bismethyl amino

RN: 59886-52-1 **MP (°C):** 220**MW:** 248.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.03E-04	<1.00E-01	rt	C317	0 0 0 0 0	

2884. C₁₂H₁₆N₄O₂S₂

Glybuthiazole

p-Aminobenzenesulfamido-*tert*-butylthiodiazole

Glipasol

Glypasol

RN: 535-65-9 **MP (°C):** 222**MW:** 312.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.820E-04	5.686E-02	37	A046	2 0 1 1 2	

2885. C₁₂H₁₆N₄O₂S₂4-Amino-*N*-(5-butyl-1,3,4-thiadiazol-2-yl)benzenesulfonamideSulfanilamide, *N*1-(5-butyl-1,3,4-thiadiazol-2-yl)-**RN:** 71119-31-8 **MP (°C):****MW:** 312.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.710E-04	8.466E-02	37	A046	2 0 1 1 2	

2886. C₁₂H₁₆N₄O₇S

2'-Methylsulfonyl-6-methoxypurine arabinoside

9H-Purine, 6-methoxy-9-[2-O-(methylsulfonyl)-β-D-arabinofuranosyl]-

RN: 145913-48-0 MP (°C): 188-190

MW: 360.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.720E-02	6.198E+00	37	C348	0 0 0 0 0	pH 7.00

2887. C₁₂H₁₆N₅O₃PS₂Azinphos-ethyl *O*-analog

RN: MP (°C):

MW: 373.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.017E-02	3.797E+00	10	B300	2 2 1 1 2	

2888. C₁₂H₁₆O*o*-Cyclohexylphenol

2-Cyclohexylphenol

RN: 119-42-6 MP (°C):

MW: 176.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.727E-04	8.333E-02	25	L021	1 0 0 0 0	

2889. C₁₂H₁₆O*p*-Cyclohexylphenol

4-Cyclohexylphenol

RN: 1131-60-8 MP (°C):

MW: 176.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.782E-04	6.666E-02	25	L021	1 0 0 0 0	

2890. C₁₂H₁₆O₂

ε-Phenylcaproic acid

6-Phenylcaproic acid

6-Phenylhexanoic acid

RN: 5581-75-9 MP (°C):

MW: 192.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.495E-03	4.798E-01	30	D033	2 2 1 2 2	
4.002E-03	7.694E-01	40	D033	2 2 1 2 2	

2891. C₁₂H₁₆O₂

4-Cyclohexylresorcinol

p-Cyclohexylresorcinol

RN: 2138-20-7 MP (°C):

MW: 192.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.599E-03	4.998E-01	25	L021	1 0 0 0 0	

2892. C₁₂H₁₆O₃

Isoamyl salicylate

Isoamyl *o*-hydroxybenzoate

3-Methylbutyl salicylate

3-Methylbutyl *o*-hydroxybenzoate

RN: 87-20-7 MP (°C):

MW: 208.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.961E-04	1.450E-01	25	D081	1 2 2 1 2	
6.918E-04	1.441E-01	ns	S460	0 0 0 0 0	

2893. C₁₂H₁₆O₇.H₂O

Arbutin (monohydrate)

Hydroquinone-β-D-glucopyranoside monohydrate

RN: 6058-77-1 MP (°C): 195–200

MW: 290.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.828E-01	1.111E+02	c	D004	0 0 0 0 0	
1.723E+00	5.000E+02	h	D004	0 0 0 0 0	

2894. C₁₂H₁₇NO₂

2,6-Diethyl-4-acetaminophenol

3,5-Diethylparacetamol

4-Acetamido-2,6-diethylphenol

RN: 55205-89-5 MP (°C):

MW: 207.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.943E-03	6.101E-01	25	D078	1 2 1 1 2	

2895. C₁₂H₁₇NO₂

Promecarb

5-Isopropyl-*m*-tolyl methylcarbamate

Carbamult

RN: 2631-37-0 **MP (°C):** 87.5
MW: 207.27 **BP (°C):** 117

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.439E-04	9.200E-02	rt	M161	0 0 0 0 1	

2896. C₁₂H₁₇NO₂Pentyl *p*-aminobenzoate

4-Aminobenzoic acid pentyl ester

RN: 13110-37-7 **MP (°C):**
MW: 207.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	8.084E-02	37	F006	1 1 2 2 1	
1.890E-04	3.917E-02	ns	M066	0 0 0 0 2	
1.890E-04	3.917E-02	rt	B016	0 0 1 1 2	pH 7.4

2897. C₁₂H₁₇NO₂2-*sec*-Butylphenyl methylcarbamate

BPMC

2-(1-Methylpropyl)phenol methylcarbamate

N-Methyl *O*-*sec*-butylphenylcarbamate

RN: 3766-81-2 **MP (°C):** 32
MW: 207.27 **BP (°C):** 112.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.294E-04	8.900E-02	22	K137	1 1 2 1 0	
3.184E-03	6.600E-01	30	M161	1 0 0 0 2	

2898. C₁₂H₁₇NO₂

Hexyl nicotinate

n-Hexyl nicotinoateNicotinic acid *n*-hexyl ester

RN: 23597-82-2 **MP (°C):**
MW: 207.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.202E-04	1.700E-01	32	L346	1 0 0 1 2	

2899. C₁₂H₁₇NO₂*m-tert-Butylphenyl N-methylcarbamate**3-tert-Butylphenyl N-methylcarbamate*

RN: 780-11-0 MP (°C): 144.0

MW: 207.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.41E-06	<5.00E-04	30	D089	2 2 0 0 0	

2900. C₁₂H₁₇NO₃*m-sec-Butoxyphenyl N-methylcarbamate**3-sec-Butoxyphenyl N-methylcarbamate*

RN: 13538-22-2 MP (°C): 53

MW: 223.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.583E-04	8.000E-02	30	D089	2 2 0 0 0	

2901. C₁₂H₁₇NO₃*m-n-Butoxyphenyl N-methylcarbamate**3-n-Butoxyphenyl N-methylcarbamate*

RN: 3978-68-5 MP (°C): 54.5

MW: 223.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.031E-04	9.000E-02	30	D089	2 2 0 0 0	

2902. C₁₂H₁₇NO₃*Acetamide, N-[4-(1-ethoxyethoxy)phenyl]-**1-(*p*-Acetaminophenoxy)-1-ethoxyethane*

RN: 51736-24-4 MP (°C):

MW: 223.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	6.698E-01	ns	H076	0 0 0 0 0	

2903. C₁₂H₁₇NO₄*3,5-Dimethoxy-acetophenetide*

RN: MP (°C):

MW: 239.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.904E-01	1.173E+02	21.80	B102	2 0 1 1 1	solid hydrate
3.344E+00	8.000E+02	35.60	B102	2 0 1 1 2	liquid hydrate
8.778E-01	2.100E+02	39.40	B102	2 0 1 1 1	solid hydrate (continued)

2903. C₁₂H₁₇NO₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.233E+00	7.736E+02	45.60	B102	2 0 1 1 2	liquid hydrate
1.586E+00	3.795E+02	57	B102	2 0 1 1 1	solid hydrate
3.172E+00	7.591E+02	58.10	B102	2 0 1 1 2	liquid hydrate
3.172E+00	7.591E+02	68.50	B102	2 0 1 1 2	liquid hydrate
2.100E+00	5.026E+02	69.50	B102	2 0 1 1 1	solid hydrate
2.288E+00	5.474E+02	72.80	B102	2 0 1 1 1	solid hydrate
2.569E+00	6.147E+02	77.10	B102	2 0 1 1 2	solid hydrate
2.790E+00	6.675E+02	80.20	B102	2 0 1 1 2	solid hydrate
2.947E+00	7.053E+02	82.60	B102	2 0 1 1 2	solid hydrate
3.049E+00	7.296E+02	84.20	B102	2 0 1 1 2	solid hydrate
3.233E+00	7.736E+02	84.30	B102	2 0 1 1 2	liquid hydrate
3.172E+00	7.591E+02	86	B102	2 0 1 1 2	solid hydrate
3.233E+00	7.736E+02	86.90	B102	2 0 1 1 2	solid hydrate
3.348E+00	8.011E+02	99.80	B102	2 0 1 1 2	liquid hydrate
3.459E+00	8.275E+02	111.10	B102	2 0 1 1 2	liquid hydrate
3.527E+00	8.440E+02	118.40	B102	2 0 1 1 2	liquid hydrate
3.632E+00	8.690E+02	129.20	B102	2 0 1 1 2	liquid hydrate
4.031E+00	9.645E+02	173.60	B102	2 0 1 1 2	liquid hydrate

2904. C₁₂H₁₇N₂O₂

4-Aminobenzoic acid-2-(propyl-amino)ethyl ester

2-(Propylamino)ethyl 4-aminobenzoate

4-Aminobenzoic acid 2-(propyl-amino)ethyl ester

RN: MP (°C):

MW: 221.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	6.638E-02	ns	M066	0 0 0 0 0	

2905. C₁₂H₁₇N₃O₄S

3'-Nitroso-tolbutamide

RN: MP (°C):

MW: 299.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.341E-04	1.000E-01	25	G051	1 0 1 1 0	

2906. C₁₂H₁₇N₅O₃

N,N-Diethylglycyloxymethyl-1-allopurinol

Glycine, N,N-diethyl-, (4,5-dihydro-4-oxo-1H-pyrazolo[3,4-d]pyrimidin-1-yl)methyl ester

RN: 98204-08-1 MP (°C):

MW: 279.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-02	4.500E+00	22	B323	0 0 0 0 0	

2907. C₁₂H₁₇O₄PS₂

Phenthaloate

Dimethyl-S-(α -ethoxycarbonylbenzyl) phosphorodithioate

Elsan

Fenthaloate

Phent

Cidial

RN: 2597-03-7 **MP (°C):**
MW: 320.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.243E-04	2.000E-01	20	M161	1 0 0 0 2	
3.434E-05	1.100E-02	22	K137	1 1 2 1 0	
3.119E-05	9.992E-03	ns	S460	0 0 0 0 0	

2908. C₁₂H₁₈

1-Phenylhexane

Hexylbenzene

n-Hexylbenzene

RN: 1077-16-3 **MP (°C):** -61
MW: 162.28 **BP (°C):** 226

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.678E-06	9.214E-04	5.04	M183	1 2 1 1 2	
5.678E-06	9.214E-04	6.04	M183	1 2 1 1 2	
5.140E-06	8.341E-04	7	O312	2 2 0 2 2	
5.667E-06	9.196E-04	8.04	M183	1 2 1 1 2	
5.583E-06	9.060E-04	9.04	M183	1 2 1 1 2	
5.150E-06	8.357E-04	10	O312	2 2 0 2 2	
5.572E-06	9.042E-04	10.04	M183	1 2 1 1 2	
5.717E-06	9.277E-04	11.04	M183	1 2 1 1 2	
5.733E-06	9.304E-04	12.04	M183	1 2 1 1 2	
5.667E-06	9.196E-04	13.04	M183	1 2 1 1 2	
5.700E-06	9.250E-04	14.04	M183	1 2 1 1 2	
5.090E-06	8.260E-04	15	O312	2 2 0 2 2	
5.594E-06	9.079E-04	15.04	M183	1 2 1 1 2	
5.661E-06	9.187E-04	16.04	M183	1 2 1 1 2	
5.606E-06	9.097E-04	17.04	M183	1 2 1 1 2	
5.678E-06	9.214E-04	18.04	M183	1 2 1 1 2	
5.811E-06	9.430E-04	19.04	M183	1 2 1 1 2	
5.860E-06	9.509E-04	20	O312	2 2 0 2 2	
5.850E-06	9.493E-04	20.04	M183	1 2 1 1 2	
5.889E-06	9.556E-04	21.04	M183	1 2 1 1 2	
5.872E-06	9.529E-04	22.04	M183	1 2 1 1 2	
6.056E-06	9.827E-04	23.04	M183	1 2 1 1 2	
6.133E-06	9.953E-04	24.04	M183	1 2 1 1 2	
6.270E-06	1.017E-03	25	M342	1 0 1 1 2	
5.560E-06	9.023E-04	25	O312	2 2 0 2 2	

(continued)

2908. C₁₂H₁₈ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.156E-06	9.989E-04	25.04	M183	1 2 1 1 2	
6.156E-06	9.989E-04	26.04	M183	1 2 1 1 2	
6.239E-06	1.012E-03	27.04	M183	1 2 1 1 2	
6.261E-06	1.016E-03	29.04	M183	1 2 1 1 2	
6.140E-06	9.964E-04	30	O312	2 2 0 2 2	
6.590E-06	1.069E-03	35	O312	2 2 0 2 2	
6.590E-06	1.069E-03	40	O312	2 2 0 2 2	
8.000E-06	1.298E-03	45	O312	2 2 0 2 2	
2.000E-03	3.246E-01	ns	H307	0 0 0 0 0	

2909. C₁₂H₁₈N₂O

Isoproturon

N,N-Dimethyl-N'-(4-(1-methylethyl)phenyl)urea

3-(4-Isopropylphenyl)-1,1-dimethylurea

Tolkan

DPX 6774

RN: 34123-59-6 MP (°C): 158.5

MW: 206.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.909E-04	6.000E-02	20	M161	1 0 0 0 1	

2910. C₁₂H₁₈N₂O₂

Zectran

4-Dimethylamino-3,5-dimethylphenol methylcarbamate ester

Mexacarbole

Mexacarbate

RN: 315-18-4 MP (°C): 85

MW: 222.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.498E-04	9.999E-02	25	I314	0 0 0 0 0	

2911. C₁₂H₁₈N₂O₂S

Thiamylal

5-Allyl-5-(1-methyl-butyl)-barbituric acid

5-Allyl-5-(1-methylbutyl)-2-thiobarbituric acid

RN: 77-27-0 MP (°C): 132

MW: 254.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.104E-03	1.298E+00	25	A023	1 0 0 1 1	
1.966E-04	5.000E-02	25	B011	2 0 0 1 0	
1.944E-04	4.946E-02	25	B065	1 1 1 1 2	

(continued)

2911. C₁₂H₁₈N₂O₂S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-04	8.852E-02	25	G003	1 1 1 1 1	pH 4.7
7.500E-03	1.908E+00	30	G014	1 1 1 1 0	EFG
6.600E-03	1.679E+00	30	I001	2 0 2 1 0	EFG, 0.003N H ₂ SO ₄
8.630E-03	2.195E+00	40	A023	1 0 0 1 1	
3.750E-03	9.538E-01	40	N008	1 2 1 1 2	<i>sic</i>
8.792E-03	2.236E+00	ns	G039	0 0 0 0 0	EFG

2912. C₁₂H₁₈N₂O₃

5-Isopropyl-5-(3-methylbut-2-enyl)barbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(3-methyl-2-butenyl)-5-(1-methylethyl)

5-*i*-Propyl-5-(3-methylbut-2-enyl)barbiturate**RN:** 67051-26-7 **MP (°C):****MW:** 238.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.555E-03	6.088E-01	25	P350	0 0 0 0 0	intrinsic

2913. C₁₂H₁₈N₂O₃

Secobarbital

5-Allyl-5-(1-methylbutyl)barbituric acid

Seconal

RN: 76-73-3 **MP (°C):** 98**MW:** 238.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.250E-03	1.728E+00	25	G003	1 1 1 1 2	pH 7
4.410E-03	1.051E+00	25	V033	2 0 1 1 2	
4.400E-03	1.048E+00	25.00	T303	1 0 0 0 1	
6.300E-03	1.501E+00	35.00	T303	1 0 0 0 1	
7.900E-02	1.882E+01	40	N008	1 0 1 1 2	<i>sic</i>
9.400E-03	2.240E+00	45.00	T303	1 0 0 0 1	

2914. C₁₂H₁₈N₂O₃S

Tolbutamide

1-Butyl-3-(*para*-tolylsulfonyl) urea

Oramide

Orinase

RN: 64-77-7 **MP (°C):** 129**MW:** 270.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.178E-04	1.400E-01	25	G051	1 0 1 1 0	
4.068E-04	1.100E-01	25	P096	0 0 0 0 0	

(continued)

2914. C₁₂H₁₈N₂O₃S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	1.054E-01	30	G318	0 0 0 0 0	EFG
4.027E-04	1.089E-01	37	A028	1 0 2 1 2	intrinsic
4.030E-04	1.090E-01	37	A046	2 0 1 1 2	
5.659E-04	1.530E-01	37	B138	1 2 0 0 2	pH 1.5, form II
5.289E-04	1.430E-01	37	B138	1 2 0 0 2	pH 1.5, form III
5.067E-04	1.370E-01	37	B138	1 2 0 0 2	pH 1.5, form I
3.699E-04	1.000E-01	37.0	H033	1 0 2 1 0	pH 1.4, intrinsic
3.031E-03	8.193E-01	37.5	F015	1 0 2 2 1	pH 6.0, pKa 5.32
2.535E-02	6.853E+00	37.5	F015	1 0 2 2 2	pH 7.0, pKa 5.32

2915. C₁₂H₁₈N₂O₄S

Anisylbutamide

Methoxyphenylbutazolamide

Methoxytolbutamide

RN: 24535-67-9 **MP (°C):**

MW: 286.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.236E-04	1.213E-01	37	A028	1 0 2 1 2	intrinsic
4.260E-04	1.220E-01	37	A046	2 0 1 1 2	

2916. C₁₂H₁₈N₂O₅

D-Mannosephenylhydrazone

D-Mannose-phenylhydrazone

RN: 6147-14-4 **MP (°C):** 195.5

MW: 270.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.811E-02	1.030E+01	100	F300	1 0 0 0 2	

2917. C₁₂H₁₈N₄O₆S

Oryzalin

3,5-Dinitro-N4,N4-dipropylsulfanilamide

RN: 19044-88-3 **MP (°C):** 137

MW: 346.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.454E-04	8.500E-02	25	B200	1 0 0 0 1	
6.929E-06	2.400E-03	25	M161	1 0 0 0 1	

2918. C₁₂H₁₈O

Propofol

2,6-Diisopropylphenol

Diisopropylphenol

Diprivan

RN: 2078-54-8 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.975E-04	1.600E-01	amb	L434	0 0 0 0 0	

2919. C₁₂H₁₈O

2-Butyl-4-ethylphenol

Phenol, 2-butyl-4-ethyl-

RN: 3781-74-6 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2920. C₁₂H₁₈O

2-Butyl-4,6-dimethylphenol

2,6-Xylenol, 2-butyl-

RN: 6483-60-9 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.603E-04	2.857E-02	25	L020	1 0 0 0 0	

2921. C₁₂H₁₈O*o-n*-Hexylphenol2-*n*-Hexylphenol

RN: 3226-32-2 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L022	1 0 0 0 0	

2922. C₁₂H₁₈O

2-Butyl-4,5-dimethylphenol

Phenol, 2-butyl-4,5-dimethyl-

RN: MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-04	3.333E-02	25	L020	1 0 0 0 0	

2923. C₁₂H₁₈O

2-Butyl-6-ethylphenol

Phenol, 2-butyl-6-ethyl-

RN: 22496-45-3 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-04	3.333E-02	25	L020	1 0 0 0 0	

2924. C₁₂H₁₈O

2,6-Dipropylphenol

Phenol, 2,6-dipropyl-

RN: 6626-32-0 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2925. C₁₂H₁₈O

4-Butyl-2,5-dimethylphenol

2,5-Xylenol, 4-butyl-

RN: 91763-77-8 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L020	1 0 0 0 0	

2926. C₁₂H₁₈O

4-Butyl-2,6-dimethylphenol

Phenol, 4-butyl-2,6-dimethyl-

2,6-Xylenol, 4-butyl-

RN: 6676-26-2 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.244E-04	4.000E-02	25	L020	1 0 0 0 0	

2927. C₁₂H₁₈O*p-n*-Hexylphenol4-*n*-Hexylphenol

RN: 2446-69-7 MP (°C):

MW: 178.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.603E-04	2.857E-02	25	L022	1 0 0 0 0	

2928. C₁₂H₁₈O

2,4-Dipropylphenol

Phenol, 2,4-dipropyl-

RN: 23167-99-9

MP (°C):

MW: 178.28

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.402E-04	2.500E-02	25	L020	1 0 0 0 0	

2929. C₁₂H₁₈O₂

4-Hexylresorcinol

4-*n*-Hexylresorcin

RN: 136-77-6

MP (°C): 68

MW: 194.28

BP (°C): 334

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.574E-03	5.000E-01	18	F300	1 0 0 0 1	

2930. C₁₂H₁₈O₄S₂

Di-isopropyl 1,3-dithiolan-2-ylidinemalonate

Isoprothiolane

Fuji-one

bis(1-Methylethyl) 1,3-dithiolan-2-ylidene propanedioate

RN: 50512-35-1 MP (°C): 52.25

MW: 290.40 BP (°C): 168

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-04	4.800E-02	20	H309	0 0 0 0 0	
1.653E-04	4.800E-02	20	M161	1 0 0 0 1	

2931. C₁₂H₁₉BrN₂O₂

Neostigmine bromide

Neostigmine bromide

Neostigmine;

Prostigmin

RN: 114-80-7 MP (°C):

MW: 303.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.298E+00	1.000E+03	ns	K444	0 0 0 0 0	

2932. C₁₂H₁₉ClNO₃P

Crufomate

O-Methyl *O*-2-chloro-4-*tert*-butyphenyl *N*-methylamidophosphate

RN: 299-86-5 **MP (°C):** 60.25
MW: 291.72 **BP (°C):** 117.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-02	4.975E+00	ns	M061	0 0 0 0 0	

2933. C₁₂H₁₉N₃O₈

Orotic acid methylglucamide

RN: **MP (°C):** 184–186
MW: 333.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.470E-01	1.490E+02	–4	N018	0 0 0 0 0	
7.090E-01	2.363E+02	16	N018	0 0 0 0 0	
8.150E-01	2.716E+02	25	N018	0 0 0 0 0	

2934. C₁₂H₁₉N₆OP

Triamiphos

5-Amino-1-(bis(dimethylamino)phosphoryl)-3-phenyl-1,2,4-triazole

Triamifos

Wepsyn 155

Wepsyn

bis(Dimethylamino)-(3-amino-5-phenyl-1,2,4-triazol-1-yl)-phosphine oxide

RN: 1031-47-6 **MP (°C):** 167.5
MW: 294.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.495E-04	2.500E-01	20	M161	1 0 0 0 2	

2935. C₁₂H₁₉O₂PS₃

Sulprofos

O-Ethyl *O*-[4-(methylthio)phenyl]phosphorodithioic acid *S*-propyl ester

Morpafos

Bolstar

Heliothion

Merdafos

RN: 35400-43-2 **MP (°C):**
MW: 322.45 **BP (°C):** 155–158

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.616E-07	3.101E-04	ns	S460	0 0 0 0 0	

2936. C₁₂H₂₀

Triisobutene

1,8-Nonadiene, 2,8-dimethyl-5-methylene-

RN: 36370-80-6 **MP (°C):****MW:** 164.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.944E-08	8.123E-06	20	B165	1 0 1 1 1	
5.838E-03	9.591E-01	97.30	B165	1 0 1 1 1	

2937. C₁₂H₂₀N₂O₃

5-Ethyl-5-n-hexylbarbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-hexyl-
Hexethal

Ortal

Ortol

RN: 77-30-5 **MP (°C):****MW:** 240.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.930E-04	2.146E-01	25	M310	2 2 2 2 2	

2938. C₁₂H₂₀N₄O₂

3-Cyclohexyl-6-dimethylamino-1-methyl-1,3,5-triazine-2,4-dione

1,3,5-Triazine-2,4(1H,3H)-dione, 3-cyclohexyl-6-(dimethylamino)-1-methyl-
Hexazinone

Pronone

DPX 3674

RN: 51235-04-2 **MP (°C):** 116**MW:** 252.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.308E-01	3.300E+01	25	M161	1 0 0 0 1	

2939. C₁₂H₂₀N₄O₆

Acetyl tetraglycine ethyl ester

Glycine, N-acetylglucylglycylglycyl-, ethyl ester

RN: 637-83-2 **MP (°C):** 264**MW:** 316.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.220E-04	2.600E-01	0	R036	0 0 0 0 0	
2.466E-03	7.800E-01	25	R036	0 0 0 0 0	
5.216E-03	1.650E+00	40	R036	0 0 0 0 0	

2940. C₁₂H₂₀O₂

Linalyl acetate

Bergamol

3,7-Dimethyl-1,6-octadien-3-yl acetate

Linalyl

RN: 115-95-7

MP (°C):

MW: 196.29

BP (°C): 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.546E-03	4.998E-01	25	M350	1 0 1 1 1	

2941. C₁₂H₂₀O₄

Dibutyl maleate

Di-*n*-butyl maleate

RN: 105-76-0

MP (°C):

MW: 228.29

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.073E-03	2.450E-01	25	F067	1 0 2 2 2	

2942. C₁₂H₂₀O₆

Tripropionin

1,2,3-Propanetriol, tripropanoate

1,2,3-Propanetriyl tripropionate

Tripropionylglycerol

Tripropanoylglycerol

RN: 139-45-7

MP (°C):

MW: 260.29

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.199E-02	3.120E+00	ns	F014	0 0 0 0 2	

2943. C₁₂H₂₁NO₈S

Topiramate

2,3:4,5-di-*O*-isopropylidene-β-D-fructopyranose sulfamate

Topamax

Tracrium

RN: 97240-79-4

MP (°C):

MW: 339.37

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.860E-02	9.705E+00	ns	S469	0 0 0 0 0	

2944. C₁₂H₂₁N₂O₃PS

Diazinon

O,O-Diethyl *O*-(2-isopropyl-6-methyl-4-pyrimidinyl), phosphorothioate

Dimpylate

Basudin

Spectracide

Fezudin

RN: 333-41-5 **MP (°C):** >120**MW:** 304.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.336E-04	7.109E-02	10	B324	0 0 0 0 0	
2.336E-04	7.110E-02	10	B324	0 0 0 0 0	
1.318E-04	4.012E-02	20	B179	0 0 0 0 0	
2.261E-04	6.881E-02	20	B300	2 1 1 1 2	
1.758E-04	5.350E-02	20	B324	0 0 0 0 0	
1.758E-04	5.350E-02	20	B324	0 0 0 0 0	
1.314E-04	4.000E-02	20	M061	1 0 0 0 1	
2.260E-04	6.880E-02	22	B169	2 1 1 1 2	
1.331E-04	4.050E-02	22	K137	1 1 2 1 0	
1.436E-04	4.370E-02	30	B324	0 0 0 0 0	
1.436E-04	4.370E-02	30	B324	0 0 0 0 0	
1.314E-04	4.000E-02	rt	M161	0 0 0 0 1	

2945. C₁₂H₂₁N₅O₂S₂

Nizatidine

Axid

N-(2-((2-((Dimethylamino)methyl)-4-thiazolyl)methyl)thio)ethyl)-*N'*-methyl-2-nitro-1,1-ethenediamine**RN:** 76963-41-2 **MP (°C):****MW:** 331.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.457E-02	2.140E+01	ns	R427	0 0 0 0 0	

2946. C₁₂H₂₁N₇O1-(4'-Formyl-1-piperazinyl)-3,5-bis(dimethylamino)-*s*-triazine

1-Piperazinecarboxaldehyde, 4-[4,6-bis(dimethylamino)-1,3,5-triazin-2-yl]-

RN: 126974-79-6 **MP (°C):****MW:** 279.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.670E-03	1.025E+00	25	B386	0 0 0 0 0	

2947. C₁₂H₂₂N₂O₂*N,N,N',N'-Tetraethylfumaramide*2-Butenediamide, *N,N,N',N'-tetraethyl-***RN:** 111328-65-5 **MP (°C):****MW:** 226.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-01	1.562E+02	30	K019	1 0 0 0 1	

2948. C₁₂H₂₂N₆*1-(Piperidinyl)-3,5-bis(dimethylamino)-s-triazine**s-Triazine, 2,4-bis(dimethylamino)-6-piperidino-***RN:** 16268-79-4 **MP (°C):****MW:** 250.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.758E-04	4.402E-02	25	B386	0 0 0 0 0	

2949. C₁₂H₂₂O₂*Arbanol***RN:** 7070-15-7 **MP (°C):****MW:** 198.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.523E-03	3.020E-01	6	P430	0 0 0 0 0	
2.911E-03	5.773E-01	23.5	P430	0 0 0 0 0	

2950. C₁₂H₂₂O₄*Ethylene glycol divalerate***RN:** **MP (°C):****MW:** 230.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.460E-04	1.488E-01	25	F064	1 0 0 0 2	

2951. C₁₂H₂₂O₄

1,10-Decanedicarboxylic acid

Decan-dicarbonsaeure-(1,10)

Dodecanedioic acid

RN: 693-23-2 MP (°C): 128

MW: 230.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-04	4.000E-02	20	F300	1 0 0 0 0	
3.039E-03	7.000E-01	21	B040	1 0 1 1 0	<i>sic</i>
5.124E-03	1.180E+00	100	F300	1 0 0 0 2	

2952. C₁₂H₂₂O₄

Dibutyl succinate

Succinic acid di-*n*-butyl ester

Tabutrex

RN: 141-03-7 MP (°C): -29

MW: 230.31 BP (°C): 108

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.984E-04	2.299E-01	ns	F014	0 0 0 0 1	

2953. C₁₂H₂₂O₆

Triethylene glycol dipropionate

Ethanol, 2,2'-[1,2-ethanediylibis(oxy)]bis-, dipropanoate

RN: 141-34-4 MP (°C):

MW: 262.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.394E-01	6.279E+01	ns	F014	0 0 0 0 2	

2954. C₁₂H₂₂O₆

Dibutyl tartrate

(2R,3R)-Di-*n*-butyl tartrate

ENT 396

RN: 87-92-3 MP (°C): 21

MW: 262.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.840E-02	4.827E+00	ns	F014	0 0 0 0 2	

2955. C₁₂H₂₂O₆

Dimethoxyethyl adipate

RN:**MW:** 262.31**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.338E-02	1.400E+01	ns	F014	0 0 0 0 2	

2956. C₁₂H₂₂O₁₁

Maltose

D-Glucose, 4-O-α-D-glucopyranosyl-

α-Maltose

Malt sugar

RN: 69-79-4**MP (°C):** 102.5**MW:** 342.30**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.166E-01	2.453E+02	0	C401	1 0 0 0 0	EFG
1.061E+00	3.631E+02	0	M043	1 0 0 0 1	
1.151E+00	3.939E+02	10	M043	1 0 0 0 1	
9.066E-01	3.103E+02	20	C401	1 0 0 0 0	EFG
1.517E+00	5.192E+02	20	D041	1 0 0 0 2	
1.280E+00	4.382E+02	20	M043	1 0 0 0 1	
1.408E+00	4.819E+02	30	M043	1 0 0 0 1	
1.124E+00	3.846E+02	40	C401	1 0 0 0 0	EFG
1.037E+00	3.548E+02	40	C401	1 0 0 0 0	EFG
1.530E+00	5.238E+02	40	M043	1 0 0 0 2	
1.252E+00	4.286E+02	60	C401	1 0 0 0 0	EFG
1.859E+00	6.364E+02	60	M043	1 0 0 0 2	
1.298E+00	4.444E+02	80	C401	1 0 0 0 0	EFG
2.191E+00	7.500E+02	80	M043	1 0 0 0 2	
1.298E+00	4.444E+02	90	C401	1 0 0 0 0	EFG
1.321E+00	4.521E+02	100	C401	1 0 0 0 0	EFG
1.517E+00	5.192E+02	rt	D021	0 0 1 1 2	

2957. C₁₂H₂₂O₁₁

β-Lactose

B-Lactose

Milchzucker

4-O-β-D-Galactopyranosyl-D-glucose

RN: 5965-66-2 **MP (°C):** 253**MW:** 342.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.525E-01	5.220E+01	20	F300	1 0 0 0 2	
7.303E-02	2.500E+01	h	F300	0 0 0 0 1	

2958. C₁₂H₂₂O₁₁

Cellobiose

4-O-β-D-Glucopyranosyl-D-glucose

4-β-D-Glucopyranosyl-D-glucopyranose

D-(+)-Cellobiose

RN: 528-50-7**MP (°C):****MW:** 342.30**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.243E-01	1.110E+02	15	F300	1 0 0 0 2	
3.475E-01	1.189E+02	30.50	M137	2 1 2 2 2	
1.198E+00	4.100E+02	h	F300	0 0 0 0 1	

2959. C₁₂H₂₂O₁₁

Lactose

4-O-B-D-Galactopyranosyl-D-glucose

Milk sugar

RN: 63-42-3**MP (°C):** 201**MW:** 342.30**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.656E-01	9.091E+01	0	C401	1 0 0 0 0	EFG
3.177E-01	1.087E+02	0	M043	1 0 0 0 2	
3.116E-01	1.067E+02	0	P052	1 0 2 2 2	
4.701E-01	1.609E+02	1	P049	1 0 1 1 1	
3.811E-01	1.304E+02	10	M043	1 0 0 0 2	
4.351E-01	1.489E+02	20	C401	1 0 0 0 0	EFG
4.767E-01	1.632E+02	20	M043	1 0 0 0 2	
5.189E-01	1.776E+02	25	D041	1 0 0 0 2	
5.470E-01	1.873E+02	25	P049	1 0 1 1 1	
6.000E-01	2.054E+02	30	D011	1 0 1 0 1	
5.880E-01	2.013E+02	30	M043	1 0 0 0 2	
5.843E-01	2.000E+02	40	C401	1 0 0 0 0	EFG
7.298E-01	2.498E+02	40	M043	1 0 0 0 2	
7.574E-01	2.593E+02	60	C401	1 0 0 0 0	EFG
1.067E+00	3.651E+02	60	M043	1 0 0 0 2	
9.738E-01	3.333E+02	80	C401	1 0 0 0 0	EFG
1.475E+00	5.050E+02	80	M043	1 0 0 0 2	
1.699E+00	5.816E+02	89	D041	1 0 0 0 2	
1.096E+00	3.750E+02	95	C401	1 0 0 0 0	EFG
1.124E+00	3.846E+02	100	C401	1 0 0 0 0	EFG
1.767E+00	6.047E+02	100	M043	1 0 0 0 2	
4.775E-01	1.635E+02	rt	D021	0 0 1 1 2	

2960. C₁₂H₂₂O₁₁

Sucrose

Saccharose

β-D-Fructofuranosyl-α-D-glucopyranoside

α-D-Glucopyranosyl β-D-fructofuranoside

Beet sugar

Cane sugar

RN: 57-50-1**MP (°C):** 191**MW:** 342.30**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (TP EAA)	Comments
1.140E+00	3.902E+02	0	C401	1 0 0 0 0	
1.878E+00	6.429E+02	0	D041	1 0 0 0 2	
1.876E+00	6.421E+02	0	G046	1 0 1 1 2	
1.142E+00	3.909E+02	0	H094	1 0 0 0 2	
1.874E+00	6.416E+02	0	M043	1 0 0 0 2	
1.884E+00	6.450E+02	0	P052	1 0 2 2 2	
1.880E+00	6.435E+02	.90	M074	1 0 0 0 2	average of 3
1.157E+00	3.961E+02	10	H094	1 0 0 0 2	
1.914E+00	6.552E+02	10	M043	1 0 0 0 2	
1.943E+00	6.650E+02	12.5	F300	1 0 0 0 2	
1.938E+00	6.633E+02	15	D041	1 0 0 0 2	
1.934E+00	6.622E+02	15.80	M074	1 0 0 0 2	average of 3
1.931E+00	6.609E+02	18.5	W013	1 2 1 1 2	
1.177E+00	4.030E+02	20	C401	1 0 0 0 0	EFG
1.203E+00	4.118E+02	20	C401	1 0 0 0 0	EFG
1.946E+00	6.660E+02	20	F300	1 0 0 0 2	
1.170E+00	4.005E+02	20	G060	1 0 0 0 2	
1.173E+00	4.015E+02	20	H094	1 0 0 0 2	
1.960E+00	6.711E+02	20	M043	1 0 0 0 2	
1.956E+00	6.697E+02	23.9	W013	1 2 1 1 2	
1.954E+00	6.689E+02	24.4	W013	1 2 1 1 2	
1.964E+00	6.723E+02	24.9	W013	1 2 1 1 2	
1.986E+00	6.798E+02	25	G046	1 0 1 1 2	
1.179E+00	4.036E+02	25	G060	1 0 0 0 2	
1.981E+00	6.779E+02	25.60	M074	1 0 0 0 2	average of 3
1.963E+00	6.721E+02	25.9	W013	1 2 1 1 2	
1.188E+00	4.067E+02	30	G060	1 0 0 0 2	
1.190E+00	4.072E+02	30	H094	1 0 0 0 2	
2.006E+00	6.865E+02	30	M043	1 0 0 0 2	
1.997E+00	6.836E+02	30.0	W013	1 2 1 1 2	
1.996E+00	6.831E+02	30.5	W013	1 2 1 1 2	
2.003E+00	6.855E+02	30.50	M074	1 0 0 0 2	average of 3
2.008E+00	6.873E+02	31.5	W013	1 2 1 1 2	
2.005E+00	6.862E+02	33.1	W013	1 2 1 1 2	
2.025E+00	6.932E+02	34.5	W013	1 2 1 1 2	
2.030E+00	6.950E+02	35	G046	1 0 1 1 2	
1.198E+00	4.100E+02	35	G060	1 0 0 0 2	
2.028E+00	6.942E+02	36.0	W013	1 2 1 1 2	
2.028E+00	6.941E+02	36.4	W013	1 2 1 1 2	
1.252E+00	4.286E+02	40	C401	1 0 0 0 0	EFG

(continued)

2960. C₁₂H₂₂O₁₁ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E+00	4.133E+02	40	G060	1 0 0 0 2	
1.207E+00	4.132E+02	40	H094	1 0 0 0 2	
2.057E+00	7.041E+02	40	M043	1 0 0 0 2	
2.050E+00	7.017E+02	40.2	W013	1 2 1 1 2	
2.052E+00	7.023E+02	40.7	W013	1 2 1 1 2	
2.055E+00	7.035E+02	41.0	W013	1 2 1 1 2	
2.061E+00	7.055E+02	42.2	W013	1 2 1 1 2	
2.067E+00	7.074E+02	42.3	W013	1 2 1 1 2	
2.080E+00	7.120E+02	45	F300	1 0 0 0 2	
1.217E+00	4.167E+02	45	G060	1 0 0 0 2	
2.093E+00	7.163E+02	46.1	W013	1 2 1 1 2	
2.107E+00	7.212E+02	49.6	W013	1 2 1 1 2	
2.111E+00	7.225E+02	50	G046	1 0 1 1 2	
1.228E+00	4.202E+02	50	G060	1 0 0 0 2	
7.596E+00	2.600E+03	50	H063	1 0 0 0 2	
1.225E+00	4.194E+02	50	H094	1 0 0 0 2	
2.101E+00	7.191E+02	50.2	W013	1 2 1 1 2	
2.118E+00	7.251E+02	51.1	W013	1 2 1 1 2	
2.124E+00	7.272E+02	52.2	W013	1 2 1 1 2	
2.126E+00	7.276E+02	52.6	W013	1 2 1 1 2	
2.134E+00	7.304E+02	53.6	W013	1 2 1 1 2	
2.134E+00	7.305E+02	53.8	W013	1 2 1 1 2	
2.126E+00	7.278E+02	54.1	W013	1 2 1 1 2	
1.237E+00	4.235E+02	55	G060	1 0 0 0 2	
2.137E+00	7.316E+02	55.8	W013	1 2 1 1 2	
2.147E+00	7.350E+02	56.1	W013	1 2 1 1 2	
2.154E+00	7.372E+02	56.4	W013	1 2 1 1 2	
2.151E+00	7.364E+02	57.5	W013	1 2 1 1 2	
2.154E+00	7.374E+02	57.8	W013	1 2 1 1 2	
2.152E+00	7.368E+02	58.4	W013	1 2 1 1 2	
2.165E+00	7.410E+02	58.6	W013	1 2 1 1 2	
2.166E+00	7.415E+02	59.7	W013	1 2 1 1 2	
1.252E+00	4.286E+02	60	C401	1 0 0 0 0	EFG
1.248E+00	4.273E+02	60	G060	1 0 0 0 2	
1.244E+00	4.259E+02	60	H094	1 0 0 0 2	
2.167E+00	7.416E+02	60	M043	1 0 0 0 2	
2.176E+00	7.448E+02	61.1	W013	1 2 1 1 2	
2.176E+00	7.447E+02	61.4	W013	1 2 1 1 2	
2.182E+00	7.469E+02	62.6	W013	1 2 1 1 2	
2.189E+00	7.493E+02	62.9	W013	1 2 1 1 2	
2.193E+00	7.505E+02	64.6	W013	1 2 1 1 2	
1.258E+00	4.307E+02	65	G060	1 0 0 0 2	
2.204E+00	7.543E+02	65.5	W013	1 2 1 1 2	
2.214E+00	7.580E+02	66.4	W013	1 2 1 1 2	
2.219E+00	7.595E+02	66.5	W013	1 2 1 1 2	
2.222E+00	7.607E+02	68.2	W013	1 2 1 1 2	
2.221E+00	7.603E+02	69.0	W013	1 2 1 1 2	
1.269E+00	4.344E+02	70	G060	1 0 0 0 2	

(continued)

2960. C₁₂H₂₂O₁₁ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.230E+00	7.632E+02	70.1	W013	1 2 1 1 2	
2.233E+00	7.645E+02	70.4	W013	1 2 1 1 2	
2.251E+00	7.706E+02	72.8	W013	1 2 1 1 2	
2.249E+00	7.698E+02	73.8	W013	1 2 1 1 2	
2.267E+00	7.760E+02	74.5	W013	1 2 1 1 2	
2.265E+00	7.752E+02	74.6	W013	1 2 1 1 2	
2.256E+00	7.724E+02	75	G046	1 0 1 1 2	
1.280E+00	4.380E+02	75	G060	1 0 0 0 2	
2.266E+00	7.758E+02	75.1	W013	1 2 1 1 2	
2.290E+00	7.840E+02	79.5	W013	1 2 1 1 2	
1.276E+00	4.366E+02	80	C401	1 0 0 0 0	EFG
1.291E+00	4.417E+02	80	G060	1 0 0 0 2	
1.090E+01	3.730E+03	80	H063	1 0 0 0 2	
2.289E+00	7.835E+02	80	M043	1 0 0 0 2	
2.304E+00	7.886E+02	82.3	W013	1 2 1 1 2	
2.333E+00	7.985E+02	85.1	W013	1 2 1 1 2	
2.335E+00	7.994E+02	85.3	W013	1 2 1 1 2	
2.337E+00	7.999E+02	85.5	W013	1 2 1 1 2	
2.344E+00	8.022E+02	86.6	W013	1 2 1 1 2	
2.346E+00	8.032E+02	88.0	W013	1 2 1 1 2	
1.298E+00	4.444E+02	90	C401	1 0 0 0 0	EFG
2.355E+00	8.061E+02	90	G046	1 0 1 1 2	
2.363E+00	8.087E+02	90.2	W013	1 2 1 1 2	
2.388E+00	8.176E+02	95	G046	1 0 1 1 2	
2.409E+00	8.247E+02	98	G046	1 0 1 1 2	
1.321E+00	4.521E+02	100	C401	1 0 0 0 0	EFG
2.424E+00	8.296E+02	100	D041	1 0 0 0 2	
2.424E+00	8.296E+02	100	G046	1 0 1 1 2	
2.424E+00	8.296E+02	100	M043	1 0 0 0 2	

2961. C₁₂H₂₃NO₃

Propylbutylaceturethane

RN: MP (°C):

MW: 229.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.395E-03	3.199E-01	20	O021	1 2 0 0 0	

2962. C₁₂H₂₃N₇

1-(4'-Methyl-1-piperizinyl)-3,5-bis(dimethylamino)-s-triazine

2-(4-Methyl-1-piperazinyl)-4,6-bis(dimethylamino)-s-triazine

RN: 5512-05-0 MP (°C):

MW: 265.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.514E-03	1.198E+00	25	B386	0 0 0 0 0	

2963. C₁₂H₂₄N₂O₂

N,N,N',N'-Tetramethylsuberamide

Octanediamide, N,N,N',N'-tetramethyl-

RN: 27397-05-3 MP (°C):

MW: 228.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.520E+00	5.754E+02	30	D010	1 2 1 1 2	

2964. C₁₂H₂₄N₃O₃PS

Thiophosphoryl trimorpholide

Morpholine, 4,4',4"-phosphinothioylidynetris-

Phosphine sulfide, trimorpholino-

RN: 14129-98-7 MP (°C):

MW: 321.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.987E-03	3.210E+00	25	A040	1 0 0 0 2	

2965. C₁₂H₂₄N₃O₄P

Phosphoryl trimorpholide

Morpholine, 4,4',4"-phosphinylidynetris-

Phosphine oxide, trimorpholino-

RN: 4441-12-7 MP (°C):

MW: 305.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.989E+00	6.072E+02	25	A040	1 0 0 0 2	

2966. C₁₂H₂₄N₆N₂,N₄,N₆-Triethyl-N₂,N₄,N₆-trimethylmelamine

1,3,5-Triazine-2,4,6-triamine, N,N',N"-triethyl-N,N',N"-trimethyl-

RN: 64124-20-5 MP (°C):

MW: 252.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.981E-04	5.000E-02	25	C051	1 2 1 1 0	pH 7

2967. C₁₂H₂₄N₉P₃

Hexaziridinocyclotriphosphazene

2,2,4,4,6,6-Hexahydro-2,2,4,4,6,6-hexakis(1-aziridinyl)-1,3,5,2,4,6-triazatriphosphorine

2,2,4,4,6,6-Hexakis(1-aziridinyl)cyclotriphosphaza-1,3,5-triene

Apholate

APN

ENT 26316

RN: 52-46-0 **MP (°C):****MW:** 387.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.582E-01	1.000E+02	ns	L076	0 1 0 0 0	approximate

2968. C₁₂H₂₄O₂

Lauric acid

Dodecanoic acid

Laurostearic acid

RN: 143-07-7 **MP (°C):** 44**MW:** 200.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.847E-04	3.700E-02	0	B136	1 0 2 1 1	
2.895E-04	5.800E-02	20	B136	1 0 2 1 1	
2.745E-04	5.500E-02	20	D041	1 0 0 0 1	
2.745E-04	5.500E-02	20.0	R001	1 1 1 1 1	
2.400E-05	4.808E-03	25	J001	1 0 2 1 2	
8.486E-06	1.700E-03	25	M083	1 0 0 1 1	
1.150E-05	2.304E-03	25	R002	0 0 0 0 0	intrinsic
2.080E-05	4.167E-03	25	R002	0 0 0 0 0	
3.345E-04	6.700E-02	30	B136	1 0 2 1 1	
3.145E-04	6.300E-02	30.0	R001	1 1 1 1 1	
3.494E-04	7.000E-02	40	B136	1 0 2 1 1	
3.844E-05	7.700E-03	40	E005	2 1 1 2 1	
3.744E-04	7.500E-02	45	B136	1 0 2 1 1	
3.744E-04	7.499E-02	45.0	R001	1 1 1 1 1	
4.593E-05	9.200E-03	50	E005	2 1 1 2 1	
5.470E-05	1.096E-02	50	J001	1 0 2 1 2	
4.343E-04	8.700E-02	60	B136	1 0 2 1 1	
5.791E-05	1.160E-02	60	E005	2 1 1 2 2	
4.343E-04	8.699E-02	60.0	R001	1 1 1 1 1	
1.847E-04	3.700E-02	.0	R001	1 1 1 1 1	

2969. C₁₂H₂₄O₂

3-Hydroxy-2,2,5,5-tetraethyltetrahydrofuran

3-Furanol, 2,2,5,5-tetraethyltetrahydro-

RN: 29839-78-9 **MP (°C):****MW:** 200.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.493E-02	2.991E+00	rt	B066	0 2 0 0 0	

2970. C₁₂H₂₄O₃

1,3-Dioxolane-4-methanol, 2-heptyl-2-methyl

2-Heptyl-4-hydroxymethyl-2-methyl-1,3-dioxolane

RN: 5660-50-4 **MP (°C):****MW:** 216.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.560E-03	7.701E-01	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

2971. C₁₂H₂₄O₄

1,3-Dioxolane-4-methanol, 2-methyl-2-[2-(pentyloxy)ethyl]

RN: 143458-56-4 **MP (°C):****MW:** 232.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.250E-02	1.452E+01	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

2972. C₁₂H₂₆

2-Methylundecane

Isododecane

RN: 31807-55-3 **MP (°C):****MW:** 170.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.174E-08	2.000E-06	25	T423	0 0 0 0 0	

2973. C₁₂H₂₆

3,3,6,6-Tetramethyloctane

RN: 62199-46-6 **MP (°C):****MW:** 170.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-07	2.100E-05	25	T423	0 0 0 0 0	

2974. C₁₂H₂₆

Dodecane

N-Dodecane

Alkane C(12)

Duodecane

Bihexyl

Adakane 12

RN: 112-40-3 **MP (°C):** -9.6
MW: 170.34 **BP (°C):** 216.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.931E-08	8.400E-06	22.5	G301	0 0 0 0 0	
2.055E-08	3.500E-06	23	C332	0 0 0 0 0	
1.068E-08	1.820E-06	25	B156	1 0 2 2 2	
4.944E-08	8.422E-06	25	F004	0 0 0 0 0	
5.871E-09	1.000E-06	25	T423	0 0 0 0 0	
3.900E-09	6.643E-07	ns	D348	0 0 0 0 0	
2.231E-08	3.800E-06	ns	H123	0 0 0 0 0	

2975. C₁₂H₂₆

2,2,4,6,6-Pentamethylheptane

RN: 13475-82-6 **MP (°C):**
MW: 170.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.468E-07	2.500E-05	25	T423	0 0 0 0 0	

2976. C₁₂H₂₆O

Dodecanol

Dodecyl alcohol

Lauryl alcohol

Undecyl carbinol

RN: 112-53-8 **MP (°C):** 24
MW: 186.34 **BP (°C):** 261

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.100E-06	1.696E-03	16	K011	1 2 1 1 2	
2.300E-05	4.286E-03	25	R002	0 0 0 0 0	
1.560E-05	2.907E-03	34	K011	1 2 1 1 2	
1.930E-05	3.596E-03	49	K011	1 2 1 1 2	

2977. C₁₂H₂₇N

Tributylamine

tris-n-Butylamine

N,N-Dibutyl-1-butanamine

RN: 102-82-9 **MP (°C):** -70
MW: 185.36 **BP (°C):** 216

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.649E-04	1.418E-01	25.04	V013	2 2 2 2 2	

2978. C₁₂H₂₇N.4H₂O

Dodecylamine (tetrahydrate)

RN: 124-22-1 **MP (°C):**
MW: 257.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.776E-03	7.145E-01	ns	R037	0 2 2 1 0	

2979. C₁₂H₂₇OP

Tributyl phosphine oxide

Tributylphosphine oxide

TBPO

RN: 814-29-9 **MP (°C):** 64
MW: 218.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E+00	2.260E+02	13.20	H031	1 2 2 2 2	
8.794E-01	1.920E+02	13.40	H031	1 2 2 2 2	
4.718E-01	1.030E+02	16.30	H031	1 2 2 2 2	
1.832E-01	4.000E+01	25	B070	1 2 0 1 1	
2.551E-01	5.570E+01	25.00	H031	1 2 2 2 2	
2.299E-01	5.020E+01	27.00	H032	1 1 2 1 2	
2.244E-01	4.900E+01	27.8	H032	1 1 2 1 2	
2.125E-01	4.640E+01	29.0	H032	1 1 2 1 2	
2.020E-01	4.410E+01	30.2	H032	1 1 2 1 2	
1.974E-01	4.310E+01	31.1	H032	1 1 2 1 2	
1.892E-01	4.130E+01	32.0	H032	1 1 2 1 2	
1.818E-01	3.970E+01	32.5	H032	1 1 2 1 2	
1.626E-01	3.550E+01	34.50	H031	1 2 2 2 2	
1.530E-01	3.340E+01	36.0	H032	1 1 2 1 2	
1.205E-01	2.630E+01	42.6	H032	1 1 2 1 2	
1.063E-01	2.320E+01	46.0	H032	1 1 2 1 2	
1.035E-01	2.260E+01	46.70	H031	1 2 2 2 2	
8.932E-02	1.950E+01	50.4	H032	1 1 2 1 2	
7.466E-02	1.630E+01	56.00	H031	1 2 2 2 2	
5.176E-02	1.130E+01	76.50	H031	1 2 2 2 2	
4.306E-02	9.400E+00	99.00	H031	1 2 2 2 2	

2980. C₁₂H₂₇O₂P

Butyl dibutyl phosphinate
 Butoxydibutylphosphine oxide
 Dibutylbutoxyphosphine oxide
 Butyl dibutylphosphinate

RN: 2950-47-2 **MP (°C):**
MW: 234.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-02	4.500E+00	25	B070	1 2 0 1 1	

2981. C₁₂H₂₇O₃P

Diethyl octyl phosphonate
 Diethyl octanephosphonate
RN: 1068-07-1 **MP (°C):**
MW: 250.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.99E-04	<2.00E-01	25	B070	1 2 0 1 0	

2982. C₁₂H₂₇O₃P

Dibutyl butyl phosphonate
 Dibutoxybutylphosphine oxide
 Dibutyl butanephosphonate
 Dibutyl butylphosphonate
 TC 44

RN: 78-46-6 **MP (°C):**
MW: 250.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.997E-03	5.000E-01	25	B070	1 2 0 1 0	

2983. C₁₂H₂₇O₄P

Tributyl phosphate
 Tri-*n*-butyl phosphate
RN: 126-73-8 **MP (°C):**
MW: 266.32 **BP (°C):** 289.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.036E-03	1.075E+00	3.4	H027	2 1 2 2 2	
3.800E-03	1.012E+00	4.0	H027	2 1 2 2 2	
3.593E-03	9.570E-01	5.0	H027	2 1 2 2 2	
2.403E-03	6.400E-01	13.0	H027	2 1 2 2 2	
1.500E-03	3.995E-01	25	B070	1 2 0 1 2	
1.464E-03	3.900E-01	25	B070	1 2 0 1 1	

(continued)

2983. C₁₂H₂₇O₄P (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.253E-02	6.000E+000	25	F300	1 0 0 0 0	
1.585E-03	4.220E-01	25.0	H027	2 1 2 2 2	
1.570E-03	4.180E-01	25.0	H032	2 2 2 1 1	
1.070E-03	2.850E-01	50.0	H027	2 1 2 2 2	EFG
1.239E-03	3.299E-01	ns	F014	0 0 0 0 1	

2984. C₁₂H₂₈Ge

Tetrapropylgermanium

Tetra-*n*-propylgermane

RN: 994-65-0 MP (°C):

MW: 244.96 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.320E-08	8.133E-06	25	D346	1 1 2 2 2	

2985. C₁₂Br₁₀O

Decabromodiphenyl ether

DBDPO

Decabromodiphenyl oxide

RN: 1163-19-5 MP (°C): 298.0

MW: 959.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.606E-08	2.500E-05	25	N326	1 0 0 0 1	average

2986. C₁₂Cl₈O₂Octachlorodibenzo-*p*-dioxin

OCDD

1,2,3,4,6,7,8,9-Octachlorodibenzodioxin

O8CDD

Octachlorodibenzo[b,e][1,4]dioxin

RN: 3268-87-9 MP (°C): 330

MW: 459.76 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-13	4.000E-10	20	F303	1 2 1 2 0	
8.700E-13	4.000E-10	20	W319	1 2 1 2 1	
1.610E-13	7.400E-11	25	S352	2 2 0 2 1	
1.610E-13	7.402E-11	25.0	D330	2 2 1 2 2	
4.350E-12	2.000E-09	40	F303	1 2 1 2 1	
4.350E-12	2.000E-09	40	W319	1 2 1 2 1	
6.750E-13	3.103E-10	40.0	D330	2 2 1 2 2	
3.960E-12	1.821E-09	60.0	D330	2 2 1 2 2	
1.710E-12	7.862E-10	80.0	D330	2 2 1 2 2	
8.374E-13	3.850E-10	ns	W332	0 1 0 2 2	

2987. C₁₂Cl₁₀

Decachlorobiphenyl

Decachlorobiphenyl

2,2',3,3',4,4',5,5',6,6'-Decachlorobiphenyl

RN: 2051-24-3 **MP (°C):** 305**MW:** 498.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.211E-11	2.100E-08	22	O311	2 2 1 2 1	
1.300E-12	6.483E-10	25	D331	2 1 2 2 2	
1.303E-11	6.500E-09	25	D335	1 0 0 0 1	
1.490E-11	7.430E-09	25	M342	1 0 1 1 2	
3.209E-11	1.600E-08	25	W025	1 0 2 2 1	
1.300E-12	6.483E-10	25.0	M324	1 2 1 1 2	
1.680E-11	8.378E-09	60	D331	2 1 2 2 2	
1.680E-11	8.378E-09	60.0	M324	1 2 1 1 2	
3.530E-11	1.760E-08	70	D331	2 1 2 2 2	
3.530E-11	1.760E-08	70.0	M324	1 2 1 1 2	
9.930E-11	4.952E-08	80	D331	2 1 2 2 2	
9.930E-11	4.952E-08	80.0	M324	1 2 1 1 2	

2988. C₁₃H₆Cl₅NO₃

Oxyclozanide

3,5,6,3',5'-Pentachloro-2,2'-dihydroxybenzamilide

Zanilox

Diplin

ICI 46638

Zanil

RN: 2277-92-1 **MP (°C):**
MW: 401.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.224E-05	2.900E-02	25	P036	0 0 0 0 0	average of 3, form III
2.665E-06	1.070E-03	25	P036	0 0 0 0 0	average of 3, form II
6.227E-07	2.500E-04	25	P036	0 0 0 0 0	average of 3, form I

2989. C₁₃H₆Cl₆O₂

Hexachlorophene

2,2'-Methylenebis[3,4,6-trichlorophenol]

Bilevon

AT-7

Dermadex

Exofene

RN: 70-30-4 **MP (°C):** 164.5
MW: 406.91 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.142E-04	2.499E-01	22	M048	1 0 1 1 0	EFG
4.669E-05	1.900E-02	25	A008	1 0 0 0 0	EFG
3.441E-04	1.400E-01	25	A010	2 2 2 1 1	0.003N HCl
7.373E-07	3.000E-04	ns	V302	0 0 0 0 0	<i>sic</i>

2990. C₁₃H₇Br₂N₃O₆

Bromofenoxim

3,5-Dibromo-4-hydroxybenzaldehyde-2,4-dinitrophenyloxime

Faneron

Bromfenim

RN: 13181-17-4 MP (°C): 196.5

MW: 461.04 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.169E-07	1.000E-04	20	M161	1 0 0 0 0	
1.288E-06	5.939E-04	ns	R427	0 0 0 0 0	

2991. C₁₃H₇F₃N₂O₅

Fluorodifen

p-Nitrophenyl α,α,α-trifluoro-2-nitro-*p*-tolyl ether

RN: 15457-05-3 MP (°C): 90

MW: 328.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.094E-06	2.000E-03	20	E048	1 2 1 1 0	
6.094E-06	2.000E-03	20	M161	1 0 0 0 0	
<6.09E-06	<2.00E-03	ns	B200	0 0 0 0 0	
6.094E-06	2.000E-03	ns	M061	0 0 0 0 0	

2992. C₁₃H₈ClFO₂

4'-Chloro-5-fluoro-2-hydroxy benzophenone

SL 79182

RN: 62433-26-5 MP (°C):

MW: 250.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.590E-05	8.999E-03	37	F309	1 0 2 2 2	

2993. C₁₃H₈CINO

CP 31675

2-Chloro-*N*-(2-methyl-6-*t*-butylphenyl)acetamide

RN: 3785-20-4 MP (°C): 115

MW: 229.67 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.306E-03	3.000E-01	ns	M061	0 0 0 0 2	

2994. C₁₃H₈ClN₃O

RJ-64

3,4-Pyridyl-(5)-2-chlorophenyl-1,2,4-oxadiazole

RN: 27199-40-2 MP (°C):

MW: 257.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.045E-03	1.300E+00	37	C054	2 2 2 1 2	0.1N HCl

2995. C₁₃H₈Cl₂N₂O₄

Niclosamide

2',5-Dichloro-4'-nitrosalicylanilide

2-Chloro-4-nitrophenylamide-6-chlorosalicylic acid

Cestocid

Devermine

Bayluscid

RN: 50-65-7 MP (°C): 230

MW: 327.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.072E-05	1.332E-02	25	T426	0 0 0 0 0	
1.987E-05	6.500E-03	rt	M161	0 0 0 0 0	

2996. C₁₃H₈F₂O₃

Diflunisal

5-(2,4-Difluorophenyl) salicylic acid

Dolobid

RN: 22494-42-4 MP (°C):

MW: 250.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.472E-05	6.186E-03	24.99	K447	0 0 0 0 0	pH 2.0
1.199E-05	3.000E-03	37	Y421	0 0 0 0 0	

2997. C₁₃H₈N₂O₂

Phenazine-1-carboxylic acid

PCA

RN: MP (°C):

MW: 224.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-04	5.157E-02	5.0	Y409	0 0 0 0 0	
2.300E-04	5.157E-02	10.0	Y409	0 0 0 0 0	
2.400E-04	5.381E-02	15.0	Y409	0 0 0 0 0	
2.500E-04	5.606E-02	20.0	Y409	0 0 0 0 0	

(continued)

2997. C₁₃H₈N₂O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	6.054E-02	25.0	Y409	0 0 0 0 0	
2.900E-04	6.502E-02	30.0	Y409	0 0 0 0 0	
3.200E-04	7.175E-02	35.0	Y409	0 0 0 0 0	
3.500E-04	7.848E-02	40.0	Y409	0 0 0 0 0	
3.900E-04	8.745E-02	45.0	Y409	0 0 0 0 0	
4.400E-04	9.866E-02	50.0	Y409	0 0 0 0 0	
5.100E-04	1.144E-01	55.0	Y409	0 0 0 0 0	

2998. C₁₃H₈N₂O₂S*m*-Pyridine carboxyphenylisothiocyanatePicolinic acid, *m*-isothiocyanatophenyl ester

RN: 5174-37-8 MP (°C):

MW: 256.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.281E-02	25	K032	2 2 0 1 1	

2999. C₁₃H₉ClN₂O₄

4'-Chloro-2-hydroxy-3-nitrobenzalide

Salicylanilide, 4'-chloro-5-nitro-

Benzamide, *N*-(4-chlorophenyl)-2-hydroxy-5nitro-

RN: 6490-98-8 MP (°C): 253–254

MW: 292.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.551E-06	2.210E-03	25	D400	2 0 0 1 2	

3000. C₁₃H₉ClN₂O₄

4'-Chloro-2-hydroxy-3-nitrobenzalide

Benzamide, *N*-(4-chlorophenyl)-2-hydroxy-3-nitro-

Salicylanilide, 4'-chloro-3-nitro-

NSC 22899

4'-Chloro-3-nitrosalicylanilide

RN: 6490-99-9 MP (°C):

MW: 292.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.851E-05	8.344E-03	25	D400	2 0 0 1 2	

3001. C₁₃H₉Cl₂NO₄

2,4-Dichlorophenyl 3-methoxy-4-nitrophenyl ether

Chlomethoxyfen

Chlomethoxynil

RN: 32861-85-1 **MP (°C):** 113.5**MW:** 314.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.550E-07	3.000E-04	15	M161	1 0 0 0 0	

3002. C₁₃H₉F₃N₂O₂

Niflumic acid

2-[3-(Trifluoromethyl)anilino]nicotinic acid

Actol

Flogovital

Donalgin

Landruma

RN: 4394-00-7 **MP (°C):** 204**MW:** 282.22 **BP (°C):** 378.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.733E-04	7.714E-02	10	B429	1 0 1 2 2	
2.805E-04	7.917E-02	15	B429	1 0 1 2 2	
2.916E-04	8.231E-02	20	B429	1 0 1 2 2	
3.028E-04	8.544E-02	25	B429	1 0 1 2 2	
3.128E-04	8.827E-02	30	B429	1 0 1 2 2	
3.261E-04	9.203E-02	35	B429	1 0 1 2 2	
6.732E-05	1.900E-02	rt	H302	0 0 2 1 1	intrinsic
1.400E-04	3.950E-02	rt	R431	0 0 0 0 0	Average

3003. C₁₃H₉N

Phenanthridine

Phenanthridin

9-Azaphenanthrene

3,4-Benzoisoquinoline

5-Azaphenanthrene

RN: 229-87-8 **MP (°C):** 106.5**MW:** 179.22 **BP (°C):** 349

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.674E-03	3.000E-01	20	F300	1 0 0 0 1	

3004. C₁₃H₉N

Acridine

2,3,5,6-Dibenzopyridine

Acridin

RN: 260-94-6 **MP (°C):** 107
MW: 179.22 **BP (°C):** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-04	5.735E-02	24	A029	2 0 0 0 1	0.01N KOH
2.142E-04	3.840E-02	24	H106	1 0 2 2 2	
2.143E-04	3.840E-02	24	M303	1 0 1 1 2	
3.348E-04	6.000E-02	30	K090	1 2 2 2 0	EFG
3.348E-04	6.000E-02	30	K090	1 2 2 2 0	

3005. C₁₃H₉NO

2-Hydroxyacridine

o-Hydroxyacridine

RN: 22817-17-0 **MP (°C):**
MW: 195.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	3.904E-03	20	A029	1 0 0 0 0	

3006. C₁₃H₉NS

p-Biphenyl isothiocyanate

4-Biphenyl isothiocyanate

RN: 25687-48-3 **MP (°C):**
MW: 211.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-05	2.958E-03	25	D019	1 1 1 1 1	

3007. C₁₃H₉NS

m-Biphenyl isothiocyanate

3-Biphenyl isothiocyanate

RN: 1510-25-4 **MP (°C):**
MW: 211.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	6.339E-03	25	K032	2 2 0 1 1	

3008. C₁₃H₁₀

Fluorene

o-Biphenylmethane

2,3-Benzindene

o-Biphenylenemethane

Diphenylenemethane

2,2'-Methylenebiphenyl

RN: 86-73-7 **MP (°C):** 116
MW: 166.22 **BP (°C):** 295

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-06	7.181E-04	6.60	M082	1 1 1 2 2	
4.320E-06	7.181E-04	6.60	M151	2 1 2 2 2	
4.326E-06	7.190E-04	6.64	M183	1 2 1 1 2	
5.820E-06	9.674E-04	13.20	M082	1 1 1 2 2	
5.820E-06	9.674E-04	13.20	M151	2 1 2 2 2	
5.822E-06	9.678E-04	13.24	M183	1 2 1 1 2	
7.240E-06	1.203E-03	18.00	M082	1 1 1 2 2	
7.240E-06	1.203E-03	18.00	M151	2 1 2 2 2	
7.244E-06	1.204E-03	18.04	M183	1 2 1 1 2	
9.012E-06	1.498E-03	20	V416	0 0 0 0 0	
9.720E-06	1.616E-03	24.00	M082	1 1 1 2 2	
9.720E-06	1.616E-03	24.00	M151	2 1 2 2 2	
9.728E-06	1.617E-03	24.04	M183	1 2 1 1 2	
1.137E-05	1.890E-03	24.60	W003	2 2 2 2 2	average of 3
1.179E-05	1.960E-03	25	B319	2 0 1 2 2	
2.790E-05	4.638E-03	25	L301	1 1 2 2 2	
1.143E-05	1.900E-03	25	L332	1 1 1 1 1	
1.191E-05	1.980E-03	25	M064	1 1 2 2 2	
1.014E-05	1.685E-03	25	M071	2 2 2 2 2	
1.190E-05	1.978E-03	25	M342	1 0 1 1 2	
1.010E-05	1.679E-03	25	W300	2 2 2 2 2	
1.014E-05	1.685E-03	25.00	M151	2 1 1 2 2	
1.110E-05	1.845E-03	27.00	M082	1 1 1 2 2	
1.110E-05	1.845E-03	27.00	M151	2 1 2 2 2	
1.111E-05	1.847E-03	27.04	M183	1 2 1 1 2	
1.420E-05	2.360E-03	29.90	W003	2 2 2 2 2	average of 3
1.317E-05	2.190E-03	30.30	W003	2 2 2 2 2	average of 3
1.350E-05	2.244E-03	31.10	M082	1 1 1 2 2	
1.350E-05	2.244E-03	31.10	M151	2 1 2 2 2	
1.353E-05	2.250E-03	31.14	M183	1 2 1 1 2	
2.244E-05	3.730E-03	38.40	W003	2 2 2 2 2	average of 2
2.223E-05	3.695E-03	40	V416	0 0 0 0 0	
2.322E-05	3.860E-03	40.10	W003	2 2 2 2 2	average of 3
3.387E-05	5.630E-03	47.50	W003	2 2 2 2 2	average of 3
3.862E-05	6.420E-03	50.10	W003	2 2 2 2 2	average of 3
3.772E-05	6.270E-03	50.20	W003	2 2 2 2 2	
5.071E-05	8.430E-03	54.70	W003	2 2 2 2 2	average of 3
6.317E-05	1.050E-02	59.20	W003	2 2 2 2 2	
5.298E-05	8.806E-03	60	V416	0 0 0 0 0	
6.678E-05	1.110E-02	60.50	W003	2 2 2 2 2	average of 3

(continued)

3008. C₁₃H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.543E-05	1.420E-02	65.10	W003	2 2 2 2 2	average of 3
1.119E-04	1.860E-02	70.70	W003	2 2 2 2 2	average of 3
1.131E-04	1.880E-02	71.90	W003	2 2 2 2 2	
1.293E-04	2.150E-02	73.40	W003	2 2 2 2 2	
1.191E-05	1.980E-03	ns	M344	0 0 0 0 2	

3009. C₁₃H₁₀BrCl₂O₂PS

Leptophos

Phenylphosphonothioic acid *O*-(4-bromo-2,5-dichlorophenyl) *O*-methyl ester

Phosvel

NK 711

Velsicol 506

Oleophosvel

RN: 21609-90-5 MP (°C): 60

MW: 412.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.280E-09	3.000E-06	10	B324	0 0 0 0 0	
8.707E-09	3.588E-06	10	B324	0 0 0 0 0	
1.699E-07	7.000E-05	20	B169	2 2 1 1 0	
6.095E-08	2.512E-05	20	B300	2 2 1 1 2	
6.095E-08	2.512E-05	20	B324	0 0 0 0 0	
5.096E-08	2.100E-05	20	B324	0 0 0 0 0	
1.141E-08	4.700E-06	20	C053	0 0 0 0 0	
1.213E-08	5.000E-06	22	K137	1 1 2 1 0	
7.280E-08	3.000E-05	24	C105	2 1 2 2 2	
5.824E-06	2.400E-03	25	M161	1 0 0 0 1	sic
1.306E-07	5.382E-05	30	B324	0 0 0 0 0	
1.092E-07	4.500E-05	30	B324	0 0 0 0 0	
2.184E-08	9.000E-06	ns	F040	1 2 2 2 0	
1.141E-08	4.700E-06	ns	F071	0 1 2 1 1	
1.699E-07	7.000E-05	ns	M110	0 0 0 0 0	EFG

3010. C₁₃H₁₀BrCl₂O₃P

Leptophos oxon

O-(4-Bromo-2,5-dichlorophenyl) *O*-methyl phenylphosphonate

Phosvel oxon

RN: 25006-32-0 MP (°C):

MW: 396.01 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.586E-06	3.400E-03	20.50	B169	2 2 1 1 2	

3011. C₁₃H₁₀ClNO₂

4'-Chloro salicylanilide

N-(*p*-Chlorophenyl)-*o*-hydroxybenzamideN-(*p*-Chlorophenyl)salicylamide**RN:** 3679-63-8 **MP (°C):****MW:** 247.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.885E-08	1.210E-05	ns	N336	0 0 0 0 0	intrinsic

3012. C₁₃H₁₀Cl₂O

2,4,-Dichloro-6-benzyl-phenol

o-Cresol, 4,6-dichloro- α -phenyl-

2-Benzyl-4,6-dichlorophenol

RN: 19578-81-5 **MP (°C):****MW:** 253.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-05	5.822E-03	25	B316	0 0 0 0 0	

3013. C₁₃H₁₀Cl₂O₂

Dichlorophen

2,2'-Dihydroxy-5,5'-dichlorodiphenylmethane

G-4

RN: 97-23-4 **MP (°C):** 177–178**MW:** 269.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.115E-04	3.000E-02	25	M061	1 0 0 0 0	
1.115E-04	3.000E-02	25	M161	1 0 0 0 1	
1.122E-04	3.020E-02	ns	R427	0 0 0 0 0	

3014. C₁₃H₁₀INO

Benodanil

2-Iodo-*N*-phenylbenzamide

Iodobenzanilide

Calirus

RN: 15310-01-7 **MP (°C):** 137**MW:** 323.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.189E-05	2.000E-02	20	M161	1 0 0 0 1	

3015. C₁₃H₁₀N₂

9-Aminoacridine

10-Amino-5-azaanthracene

Monocrin

Izoacridina

Aminacrine

9AA

RN: 90-45-9**MP (°C):** 241**MW:** 194.24**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.165E-02	24	A029	2 0 0 1 0	0.01N KOH

3016. C₁₃H₁₀N₂

4-Aminoacridine

4-Acridinamine

RN: 578-07-4**MP (°C):** 108.5**MW:** 194.24**BP (°C):** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.360E-02	24	A029	2 0 0 1 0	0.01N KOH

3017. C₁₃H₁₀N₂

3-Aminoacridine

3-Acridinamine

RN: 581-29-3**MP (°C):** 108.5**MW:** 194.24**BP (°C):** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	2.914E-02	24	A029	2 0 0 1 1	0.01N KOH

3018. C₁₃H₁₀N₂

2-Aminoacridine

2-Acridinamine

RN: 581-28-2**MP (°C):** 108.5**MW:** 194.24**BP (°C):** 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	9.712E-03	24	A029	2 0 0 1 0	0.01N KOH

3019. C₁₃H₁₀N₂

1-Aminoacridine

1-Acridinamine

RN: 578-06-3

MP (°C): 183

MW: 194.24

BP (°C): 346

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.165E-02	24	A029	2 0 0 0 1	intrinsic

3020. C₁₃H₁₀N₄O₃

1-Benzoyloxymethyl allopurinol

4H-Pyrazolo[3,4-d]pyrimidin-4-one, 1-[(benzoyloxy)methyl]-1,5-dihydro-

RN: 98846-65-2 MP (°C): 217–219

MW: 270.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.881E-05	2.400E-02	22	B322	0 0 0 0 0	
8.913E-05	2.409E-02	ns	R427	0 0 0 0 0	

3021. C₁₃H₁₀O

Benzophenone

α-Oxodiphenylmethane

Diphenylmethanone

Benzoylbenzene

α-Oxoditane

Oxoditane

RN: 119-61-9

MP (°C): 48.5

MW: 182.22

BP (°C): 305.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.121E-04	7.510E-02	20	H301	0 0 0 0 0	
7.500E-04	1.367E-01	25	F063	1 1 0 0 1	
3.292E-04	6.000E-02	ns	F014	0 0 0 0 0	

3022. C₁₃H₁₀O₃

2,4-Dihydroxybenzophenone

RN: 131-56-6 MP (°C):

MW: 214.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.291E-02	7.050E+00	19.99	L452	0 0 0 0 0	
4.255E-02	9.116E+00	24.99	L452	0 0 0 0 0	
4.805E-02	1.029E+01	29.99	L452	0 0 0 0 0	
5.672E-02	1.215E+01	34.99	L452	0 0 0 0 0	
7.396E-02	1.584E+01	39.99	L452	0 0 0 0 0	

(continued)

3022. C₁₃H₁₀O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.659E-02	1.855E+01	44.99	L452	0 0 0 0 0	
1.174E-01	2.515E+01	49.99	L452	0 0 0 0 0	
1.500E-01	3.213E+01	54.99	L452	0 0 0 0 0	
1.925E-01	4.123E+01	59.99	L452	0 0 0 0 0	
2.559E-01	5.482E+01	64.99	L452	0 0 0 0 0	
3.498E-01	7.493E+01	69.99	L452	0 0 0 0 0	

3023. C₁₃H₁₀O₃

Phenyl salicylate

Salol

2-Hydroxybenzoic acid phenyl ester

RN: 118-55-8 MP (°C): 42.0
 MW: 214.22 BP (°C): 173.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.002E-04	1.500E-01	25	F300	1 0 0 0 1	
7.469E-05	1.600E-02	ns	B404	0 2 1 1 0	
1.866E-03	3.998E-01	rt	D021	0 0 1 1 0	

3024. C₁₃H₁₀O₄

2,3,4-Trihydroxybenzophenone

2,3,4-Trihydroxy-benzophenon

RN: 1143-72-2 MP (°C):
 MW: 230.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.811E-02	1.108E+01	19.99	L452	0 0 0 0 0	
5.743E-02	1.322E+01	24.99	L452	0 0 0 0 0	
8.057E-02	1.855E+01	29.99	L452	0 0 0 0 0	
1.051E-01	2.420E+01	34.99	L452	0 0 0 0 0	
1.392E-01	3.204E+01	39.99	L452	0 0 0 0 0	
1.831E-01	4.215E+01	44.99	L452	0 0 0 0 0	
2.574E-01	5.927E+01	49.99	L452	0 0 0 0 0	
3.440E-01	7.919E+01	54.99	L452	0 0 0 0 0	
4.723E-01	1.087E+02	59.99	L452	0 0 0 0 0	
6.152E-01	1.416E+02	64.99	L452	0 0 0 0 0	
7.804E-01	1.797E+02	69.99	L452	0 0 0 0 0	

3025. C₁₃H₁₀O₄

2,4,6-Trihydroxybenzophenone

2,4,6-Trihydroxy-benzophenon

RN: 3555-86-0 MP (°C):

MW: 230.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.347E-02	3.100E+00	22	F300	1 0 0 0 1	

3026. C₁₃H₁₀O₅

2,2',4,4'-Tetrahydroxybenzophenone

RN: MP (°C):

MW: 246.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.863E-02	7.050E+00	19.99	L452	0 0 0 0 0	
3.583E-02	8.821E+00	24.99	L452	0 0 0 0 0	
4.538E-02	1.117E+01	29.99	L452	0 0 0 0 0	
6.199E-02	1.526E+01	34.99	L452	0 0 0 0 0	
8.431E-02	2.076E+01	39.99	L452	0 0 0 0 0	
1.079E-01	2.657E+01	44.99	L452	0 0 0 0 0	
1.487E-01	3.661E+01	49.99	L452	0 0 0 0 0	
2.190E-01	5.393E+01	54.99	L452	0 0 0 0 0	
3.285E-01	8.088E+01	59.99	L452	0 0 0 0 0	
4.448E-01	1.095E+02	64.99	L452	0 0 0 0 0	
5.572E-01	1.372E+02	69.99	L452	0 0 0 0 0	

3027. C₁₃H₁₀O₅

2,3,4,4'-Tetrahydroxybenzophenone

RN: 31127-54-5 MP (°C):

MW: 246.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.578E-02	1.127E+01	19.99	L452	0 0 0 0 0	
6.120E-02	1.507E+01	24.99	L452	0 0 0 0 0	
8.820E-02	2.172E+01	29.99	L452	0 0 0 0 0	
1.202E-01	2.960E+01	34.99	L452	0 0 0 0 0	
1.712E-01	4.215E+01	39.99	L452	0 0 0 0 0	
2.299E-01	5.660E+01	44.99	L452	0 0 0 0 0	
3.216E-01	7.919E+01	49.99	L452	0 0 0 0 0	
4.768E-01	1.174E+02	54.99	L452	0 0 0 0 0	
6.166E-01	1.518E+02	59.99	L452	0 0 0 0 0	
8.432E-01	2.076E+02	64.99	L452	0 0 0 0 0	
1.084E+00	2.669E+02	69.99	L452	0 0 0 0 0	

3028. C₁₃H₁₀O₆

Maclurin

2,4,6,3',4'-Penta-hydroxy-benzophenol

2,4,6,3',4'-Pentahydroxybenzophenone

RN: 519-34-6 **MP (°C):** 222.5**MW:** 262.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-02	5.000E+00	14	F300	1 0 0 0 0	

3029. C₁₃H₁₁ClF₃N₃O

San 6706

4-Chloro-5-(dimethylamino)-2-(α,α,α-trifluoro-*m*-tolyl)-3(2H)-pyridazinone**RN:** 23576-23-0 **MP (°C):** 151**MW:** 317.70 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.305E-05	1.050E-02	23.50	B200	2 0 0 0 2	

3030. C₁₃H₁₁CIN₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-

RN: 134698-40-1 **MP (°C):****MW:** 274.71 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-06	1.199E-03	ns	M381	0 1 1 1 2	pH 7.0

3031. C₁₃H₁₁ClO

Chlorophene

5-Chloro-2-hydroxydiphenylmethane

Benzylchlorophenol

RN: 120-32-1 **MP (°C):** 48.5**MW:** 218.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-02	4.155E+00	20	A008	1 0 0 0 0	EFG
1.100E-01	2.406E+01	ns	B047	0 0 0 0 0	EFG

3032. C₁₃H₁₁N

2-Aminofluorene

9H-Fluoren-2-amine

2-Fluorenamine

RN: 153-78-6 MP (°C): 129

MW: 181.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	3.100E-02	rt	N015	0 0 2 2 1	

3033. C₁₃H₁₁NO₂

Salicylanilide

2-Hydroxy-N-phenylbenzamide

2-Hydroxybenzanilide

RN: 87-17-2 MP (°C): 136

MW: 213.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.579E-04	5.500E-02	23	M061	1 0 0 0 1	
2.579E-04	5.500E-02	25	M161	1 0 0 0 1	

3034. C₁₃H₁₁NO₃

Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1,7-dimethyl-

RN: 74103-12-1 MP (°C):

MW: 229.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.597E-08	2.200E-05	25	P089	0 0 0 0 0	
1.527E-07	3.500E-05	37	P089	0 0 0 0 0	
2.116E-07	4.850E-05	51	P089	0 0 0 0 0	

3035. C₁₃H₁₁NO₃

Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1,6-dimethyl-

RN: MP (°C):

MW: 229.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-07	5.800E-05	25	P089	0 0 0 0 0	
3.054E-07	7.000E-05	37	P089	0 0 0 0 0	
3.817E-07	8.750E-05	51	P089	0 0 0 0 0	

3036. C₁₃H₁₁NO₅

Oxolinic acid

5-Ethyl-5,8-dihydro-8-oxo-1,3-dioxolo(4,5-g)quinoline-7-carboxylic acid

Dioxacin

Gramurin

Starner

S-0208

RN: 14698-29-4 **MP (°C):****MW:** 261.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-05	3.214E-03	ns	R427	0 0 0 0 0	

3037. C₁₃H₁₁N₃O₂

Benquinox

Cerenox

Seredon

Benzoylhydrazone of quinone oxime

RN: 495-73-8 **MP (°C):****MW:** 241.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.073E-05	5.000E-03	ns	M061	0 0 0 0 0	

3038. C₁₃H₁₁N₃O₂S₂

2-Sulfanilamidobenzothiazole

RN: **MP (°C):****MW:** 305.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.275E-06	1.000E-03	37	R045	1 2 1 1 1	

3039. C₁₃H₁₁N₃O₄S₂

Tenoxicam

Mobiflex

RN: 59804-37-4 **MP (°C):****MW:** 337.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.835E-04	6.190E-02	32	C411	2 1 1 2 1	

3040. C₁₃H₁₁N₇O₄S

5-p-Nitrobenzenesulfonamidotetrazole

RN: **MP (°C):**
MW: 361.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.214E-05	8.000E-03	37	R045	1 2 1 1 0	

3041. C₁₃H₁₁O₃P

4-Carboxyethylphenylphenylphosphinic acid

CPPPA

RN: **MP (°C):**
MW: 246.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.399E-02	3.443E+00	-239.0	W412	0 0 0 0 0	
1.242E-02	3.059E+00	26.7	W412	0 0 0 0 0	
1.676E-02	4.127E+00	45.08	W412	0 0 0 0 0	
1.931E-02	4.754E+00	54.4	W412	0 0 0 0 0	
2.609E-02	6.424E+00	64.15	W412	0 0 0 0 0	
3.477E-02	8.561E+00	75.71	W412	0 0 0 0 0	
4.371E-02	1.076E+01	84.38	W412	0 0 0 0 0	
3.780E+00	9.307E+02	94.52	W412	0 0 0 0 0	

3042. C₁₃H₁₂

Diphenylmethane

1,1'-Methylenebis-benzene

Phenylbenzyl

Benzylbenzene

RN: 101-81-5 **MP (°C):** 25.9
MW: 168.24 **BP (°C):** 264.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-05	3.000E-03	24	H116	2 1 0 0 2	
8.381E-05	1.410E-02	25	A001	1 2 2 2 2	
8.381E-05	1.410E-02	25	A017	1 0 0 0 2	
8.710E-05	1.465E-02	25	D001	1 0 0 0 2	

3043. C₁₃H₁₂

4-Methylbiphenyl

4-Phenyltoluene

RN: 644-08-6

MP (°C): 49.5

MW: 168.24

BP (°C): 267.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-05	1.834E-03	4.9	D330	2 2 1 2 2	
2.410E-05	4.055E-03	25.0	D330	2 2 1 2 2	
4.180E-05	7.032E-03	40.0	D330	2 2 1 2 2	

3044. C₁₃H₁₂F₂N₆O

Fluconazole

1H-1,2,4-Triazole-1-ethanol, α(2,4-difluorophenyl)-α-(1H-1,2,4-triazol-1-ylmethyl)

2,4-Difluoro-α,α1-bis(1H-1,2,4-triazol-1-ylmethyl)benzyl alcohol

Diflucan

Triflucan

RN: 86386-73-4

MP (°C): 138–140

MW: 306.28

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.265E-03	1.000E+00	ns	K444	0 0 0 0 0	

3045. C₁₃H₁₂N₂O

Carbanilide

Diphenylurea

N,N'-Diphenylurea

RN: 102-07-8

MP (°C): 238.0

MW: 212.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.079E-04	1.503E-01	ns	R427	0 0 0 0 0	
7.066E-04	1.500E-01	rt	D021	0 0 1 1 1	

3046. C₁₃H₁₂N₂O₃

Phenallymal

5-Allyl-5-phenylbarbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-phenyl-5-(2-propenyl)

Barbituric acid, 5-allyl-5-phenyl

5-Allyl-5-phenylbarbiturate

RN: 115-43-5

MP (°C): 156.5

MW: 244.25

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.499E-03	1.099E+00	20	J030	1 2 2 2 2	
4.272E-03	1.043E+00	25	P350	0 0 0 0 0	intrinsic
7.764E-03	1.896E+00	37	J030	1 2 2 2 2	

3047. C₁₃H₁₂N₂O₅S

Nimesulide

N-(4-Nitro-2-phenoxyphenyl)-methanesulfonamide

RN: 51803-78-2 MP (°C):

MW: 308.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.541E-05	1.400E-02	25	S415	0 0 0 0 0	
7.395E-05	2.280E-02	37	P432	0 0 0 0 0	

3048. C₁₃H₁₂O*p*-Benzylphenol

4-Benzylphenol

RN: 101-53-1 MP (°C): 81.5

MW: 184.24 BP (°C): 322

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.427E-04	9.999E-02	25	L021	1 0 0 0 0	

3049. C₁₃H₁₂O*o*-Benzylphenol

2-Benzylphenol

RN: 28994-41-4 MP (°C): 53.5

MW: 184.24 BP (°C): 312

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.085E-03	2.000E-01	25	L021	1 0 0 0 0	

3050. C₁₃H₁₂O

Benzhydrol

Diphenylmethanol

RN: 91-01-0 MP (°C): 69

MW: 184.24 BP (°C): 298

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.714E-03	5.000E-01	20	F300	1 0 0 0 0	
2.800E-03	5.159E-01	25	D007	2 0 1 1 1	

3051. C₁₃H₁₂O₅

bis(4-Hydroxy-3-coumarin) acetic acid ethyl ester

RN: 548-00-5 **MP (°C):**
MW: 248.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.188E-04	5.431E-02	ns	R427	0 0 0 0 0	

3052. C₁₃H₁₃Cl₂N₃O₃

Glycophen

1-Imidazolidinecarboxamide, 3-(3,5-dichlorophenyl)-N-(1-methylethyl)-2,4-dioxo-

Iprodial

LFA 2043

Iprodione

RN: 36734-19-7 **MP (°C):** 136
MW: 330.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.937E-05	1.300E-02	20	M161	1 0 0 0 1	

3053. C₁₃H₁₃NO₂

α-(β-Naphthyl)-α-alanine

Alanine, 3-(1(4H)-naphthylidene)-

RN: 13913-40-1 **MP (°C):**
MW: 215.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.260E-03	4.865E-01	25	M097	2 2 2 2 2	

3054. C₁₃H₁₃NO₅

2-Azetidinecarboxylic acid, 1-[(benzoyloxy)acetyl]-

RN: 115178-74-0 **MP (°C):** 149.5
MW: 263.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.217E-03	1.900E+00	22	N317	1 1 2 1 2	

3055. C₁₃H₁₃N₃O₃S

N4-Acetyl sulfapyridine
Acetylsulfapyridine
Sulfapyridine acetylene

RN: 19077-98-6 **MP (°C):**
MW: 291.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.098E-03	3.200E-01	37	D084	1 0 1 0 1	
7.207E-04	2.100E-01	37	F075	1 0 2 2 2	
1.119E-03	3.260E-01	37	M057	1 0 0 0 2	pH 5.5

3056. C₁₃H₁₃N₃O₅S₂

Succinylsulfathiazole
2-(N(4)-Succinylsulfanilamido)thiazole
p-2-Thiazolylsulfamoylsuccinanilic acid
Kaoxidin
Colistatin
Cremosuxidine

RN: 116-43-8 **MP (°C):**
MW: 355.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-03	4.900E-01	38	K006	1 0 0 0 1	

3057. C₁₃H₁₃O₄P

Diphenyl methyl phosphate
Methyl diphenyl phosphate

RN: 115-89-9 **MP (°C):**
MW: 264.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.633E-06	9.600E-04	24	H116	2 1 0 0 2	<i>sic</i>
7.569E-03	2.000E+00	25	A044	1 0 0 0 0	<i>sic</i>

3058. C₁₃H₁₄

1,4,5-Trimethylnaphthalene
Naphthalene, 1,4,5-trimethyl-

RN: 2131-41-1 **MP (°C):** 58
MW: 170.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-05	2.100E-03	25	M064	1 1 2 2 1	
1.190E-05	2.026E-03	25	M342	1 0 1 1 2	
1.233E-05	2.100E-03	ns	M344	0 0 0 0 1	

3059. C₁₃H₁₄F₃N₃O₄

Ethalfluralin

N-Ethyl-N-(2-methyl-2-propenyl)-2,6-dinitro-4-(trifluoromethyl)benzenamine

Buvilan

Solanan

RN: 55283-68-6 MP (°C): 55.5

MW: 333.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.001E-07	2.000E-04	25	M161	1 0 0 0 0	pH 7
9.002E-07	3.000E-04	ns	D304	1 0 0 0 0	

3060. C₁₃H₁₄N₂

4,4'-Methylenedianiline

4,4'-Methylenebisbenzeneamine

Tinox

HT 972

RN: 101-77-9 MP (°C): 93

MW: 198.27 BP (°C): 398

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.044E-03	1.000E+00	19	I307	0 0 0 0 0	

3061. C₁₃H₁₄N₂O₃

Mephobarital

5-Ethyl-1-methyl-5-phenylbarbituric acid

5-Ethyl-N-methyl-5-phenylbarbituric acid

Mebaral

Prominal

Methylphenobarbital

RN: 115-38-8 MP (°C): 176

MW: 246.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.090E-04	1.500E-01	20	J030	1 2 2 2 1	
4.872E-04	1.200E-01	37	J030	1 2 2 2 1	

3062. C₁₃H₁₄N₂O₆

Benzoic acid, 2-(acetyloxy)-, 2-[(2-amino-2-oxoethyl)amino]-2-oxoethyl ester

RN: 118247-02-2 MP (°C): 186

MW: 294.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.990E-03	8.800E-01	21	N335	0 0 0 0 0	

3063. C₁₃H₁₄N₄Pyridine-2-azo-*p*-dimethylaniline

PADA

2-(*p*-*N,N*-Dimethylaminophenylazo)pyridine*p*-(2-Pyridylazo)-*N,N*-dimethylaniline*N,N*-Dimethyl-4-(2-pyridylazo)aniline2-(*p*-*N,N*-Dimethylaminophenylazo)pyridine**RN:** 13103-75-8 **MP (°C):****MW:** 226.28 **BP (°C):** 392.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-05	2.127E-02	ns	B418	0 2 1 1 2	

3064. C₁₃H₁₄N₄O₃S

N4-Acetylsulfamerazine

N4-Acetylsulphamerazine

2-N4-Acetylsulfanilamido-4-methylpyrimidine

RN: 127-73-1 **MP (°C):****MW:** 306.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-03	3.676E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
2.579E-03	7.900E-01	37	L091	1 0 0 0 1	pH 5.5
9.140E-04	2.800E-01	37	R045	1 2 1 1 2	
9.140E-04	2.800E-01	37	R045	1 2 1 1 1	
1.234E-03	3.780E-01	37	S192	1 0 1 1 2	pH 6.0
2.611E-03	8.000E-01	38	K006	1 0 0 0 1	

3065. C₁₃H₁₄N₄O₄S

Acetyl sulfamethoxypyridazine

3-(*N*1-Acetylsulfanilamido)-6-methoxypyridazine

Acetylmidicel

RN: 127-75-3 **MP (°C):****MW:** 322.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.825E-04	2.200E-01	37	B046	1 0 2 2 1	pH 4.5

3066. C₁₃H₁₄O₆

Salicylic acid acetate, hydroxymethyl ester propionate

RN: 32620-70-5 **MP (°C):** 51.5**MW:** 266.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.629E-03	7.000E-01	21	N335	0 0 0 0 0	

3067. C₁₃H₁₄O₆

Methylphthalyl ethyl glycolate

2-Ethoxy-2-oxoethyl methyl ester

RN: 85-71-2 **MP (°C):** <-35
MW: 266.25 **BP (°C):** 189

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-03	5.297E-01	20	F070	1 0 0 0 2	

3068. C₁₃H₁₅NO₂

Glutethimide

Doriden

Noxyron

RN: 77-21-4 **MP (°C):** 84
MW: 217.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.372E-03	9.500E-01	27	B043	1 0 1 2 0	EFG
4.600E-03	9.994E-01	30	D010	1 2 1 1 2	
4.603E-03	1.000E+00	32	B043	1 0 1 2 0	EFG
5.753E-03	1.250E+00	37	B043	1 0 1 2 0	EFG
5.523E-05	1.200E-02	37	B045	1 0 1 1 2	
4.603E-03	1.000E+00	ns	A090	0 0 0 0 1	sic
4.600E-03	9.994E-01	ns	R010	0 1 0 0 2	

3069. C₁₃H₁₅NO₂

Pyracarbolid

3,4-Dihydro-6-methyl-N-phenyl-2H-pyran-5-carboxamide

Sicarol

RN: 24691-76-7 **MP (°C):** 110.5
MW: 217.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.762E-03	6.000E-01	40	M161	1 0 0 0 0	

3070. C₁₃H₁₅NO₂S

m-Carboxypentylphenylisothiocyanate

RN: **MP (°C):**
MW: 249.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-05	1.820E-02	25	K032	2 2 0 1 1	

3071. C₁₃H₁₅NO₃

Pyrrolidine, 1-[(benzoyloxy)acetyl]-
RN: 115178-67-1 **MP (°C):** 58
MW: 233.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.701E-02	6.300E+00	22	N317	1 1 2 1 2	

3072. C₁₃H₁₅NO₄

Morpholine, 4-[(benzoyloxy)acetyl]-
RN: 106231-68-9 **MP (°C):** 103.5
MW: 249.27 **BP (°C):** 453.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.685E-02	4.200E+00	22	B427	1 0 0 1 1	
1.685E-02	4.200E+00	22	N317	1 1 2 1 2	

3073. C₁₃H₁₅NO₅

Benzoic acid, 2-(acetyloxy)-, 2-(dimethylamino)-2-oxoethyl ester
RN: 118247-04-4 **MP (°C):** 75.5
MW: 265.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-02	7.500E+00	21	N335	0 0 0 0 0	

3074. C₁₃H₁₅NO₅

Benzoic acid, 2-(acetyloxy)-, 2-(ethylamino)-2-oxoethyl ester
RN: 118247-01-1 **MP (°C):** 80.5
MW: 265.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-02	5.520E+00	21	N335	0 0 0 0 0	

3075. C₁₃H₁₅N₃O₂

Pyrolan
1-Phenyl-3-methylpyrazolyl-5-dimethylcarbamate
RN: 87-47-8 **MP (°C):** 50
MW: 245.28 **BP (°C):** 161

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.138E-03	1.996E+00	ns	M061	0 0 0 0 0	

3076. C₁₃H₁₅N₃O₃S

2-Sulfanilamido-3-ethoxypyridine

Benzenesulfonamide, 4-amino-*N*-(3-ethoxy-2-pyridinyl)-**RN:** 71119-19-2 **MP (°C):****MW:** 293.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.011E-04	2.350E-01	37	R058	1 2 1 1 2	

3077. C₁₃H₁₅N₃O₃S

5-Sulfanilamido-2-ethoxypyridine

Benzenesulfonamide, 4-amino-*N*-(6-ethoxy-3-pyridinyl)-**RN:** 71720-65-5 **MP (°C):****MW:** 293.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.227E-04	3.600E-02	37	R058	1 2 1 1 1	

3078. C₁₃H₁₅N₃O₄S

Acetyl sulfisoxazole

*N*1-Acetyl-sulfaisoxazole**RN:** 80-74-0 **MP (°C):** 193.5**MW:** 309.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.586E-04	8.000E-02	37	B046	1 0 2 2 0	pH 4.5
1.199E-04	3.710E-02	37	M117	2 1 1 1 2	pH 6.0

3079. C₁₃H₁₅N₃O₄S*N*1-(3,4-Dimethyl-5-isoxazolyl)-*N*4-acetylsulfanilamide

Acetylsulfadimethylisoxazole

*N*4-Acetyl sulfisoxazole4-*N*-Acetyl sulfisoxazole*N*-Acetyl sulfisoxazole**RN:** 4206-74-0 **MP (°C):****MW:** 309.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.450E-02	7.579E+00	37	B110	1 0 2 2 2	pH 6.7

3080. C₁₃H₁₆Cl₂O₃

2,4-Dichlorophenoxyacetic acid 1-ethylpropyl ester

RN: 65267-94-9 **MP (°C):****MW:** 291.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.667E-05	4.855E-03	ns	M120	0 0 1 1 2	

3081. C₁₃H₁₆Cl₂O₃2,4-Dichlorophenoxyacetic acid *n*-pentyl ester

2,4-D Pentyl ester

Pentyl 2,4-dichlorophenoxyacetate

Amyl 2,4-dichlorophenoxyacetate

RN: 1917-92-6 **MP (°C):****MW:** 291.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.897E-05	8.436E-03	ns	M120	0 0 1 1 2	

3082. C₁₃H₁₆Cl₂O₃

2,4-Dichlorophenoxyacetic acid 2-methylbutyl ester

RN: **MP (°C):****MW:** 291.18 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.291E-05	3.760E-03	ns	M120	0 0 1 1 2	

3083. C₁₃H₁₆F₃N₃O₄

Benefin

Benfluralin

RN: 1861-40-1 **MP (°C):** 65**MW:** 335.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.98E-06	<1.00E-03	25	B200	1 0 0 0 0	
<2.98E-06	<1.00E-03	25	M161	1 0 0 0 0	
<2.98E-06	<1.00E-03	25	P028	0 0 0 0 0	
2.088E-04	7.000E-02	ns	M061	0 0 0 0 1	

3084. C₁₃H₁₆F₃N₃O₄

Trifluralin

 α,α,α -Trifluoro-2,6-dinitro-*N,N*-dipropyl-*p*-toluidine**RN:** 1582-09-8 **MP (°C):** 48.5**MW:** 335.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.193E-05	4.000E-03	20	F311	1 2 2 2 1	
2.419E-05	8.110E-03	22	K137	1 1 2 1 0	
1.730E-06	5.800E-04	25	G319	0 0 0 0 0	
<2.98E-06	<1.00E-03	27	B200	1 0 0 0 0	
<2.98E-06	<1.00E-03	27	M161	1 0 0 0 0	
<2.98E-06	<1.00E-03	27	P028	0 0 0 0 0	
7.158E-05	2.400E-02	ns	B185	0 0 0 0 0	
1.193E-04	4.000E-02	ns	M061	0 0 0 0 1	
2.088E-06	7.000E-04	ns	M110	0 0 0 0 0	
5.488E-07	1.840E-04	ns	V414	0 0 0 0 0	EFG

3085. C₁₃H₁₆NO₄PS

Isoxathion

O,O-Diethyl *O*-5-phenylisoxazol-3-yl phosphorothioate

E-48

Karphos

SI-6711

RN: 18854-01-8 **MP (°C):****MW:** 313.31 **BP (°C):** 160

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.064E-06	1.900E-03	25	N305	1 0 0 0 1	

3086. C₁₃H₁₆N₂

3-(1-Methyl-2-pyrrolidinyl)-indole

RN: **MP (°C):****MW:** 200.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.510E-03	7.030E-01	37	H004	0 0 0 0 0	
3.510E-03	7.030E-01	37	H011	0 0 0 0 0	

3087. C₁₃H₁₆N₂O₂

Melatonin

Prime-X

RN: 8041-44-9 **MP (°C):****MW:** 232.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-03	4.344E-01	25	B426	1 1 2 2 2	

3088. C₁₃H₁₆N₂O₄

N-Acetyl-L-tyrosinamide acetate

RN: MP (°C):
MW: 264.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-02	3.436E+00	25	A066	1 0 1 1 1	

3089. C₁₃H₁₆N₂O₄

Methyl-2-ethyl-2-phenylmalonurate

Methyl 2-ethyl-2-phenylmalonurate

RN: 73632-81-2 MP (°C): 105
MW: 264.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	4.757E-01	23	B152	1 2 1 1 1	pH 3.5

3090. C₁₃H₁₆N₂O₆

Medinoterb acetate

m-Cresol, 6-*tert*-butyl-2,4-dinitro-, acetate

MC 1488

RN: 2487-01-6 MP (°C): 86.5
MW: 296.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.375E-05	1.000E-02	rt	M161	0 0 0 0 1	

3091. C₁₃H₁₆N₄O₂S

2-Sulfanilylamoно-4-ethyl-5-methylpyrimidine

RN: MP (°C):
MW: 292.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.551E-04	2.500E-01	37	R076	1 2 0 0 1	

3092. C₁₃H₁₆N₄O₂S2-*p*-Aminobenzenesulphonamido-4,5,6-trimethylpyrimidineSulfanilamide, *N*1-(4,5,6-trimethyl-2-pyrimidinyl)-

RN: 5433-64-7 MP (°C):
MW: 292.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.131E-04	1.500E-01	37	R075	1 0 0 0 1	

3093. C₁₃H₁₆N₄O₆.0.5H₂O

9-[5-O-(Acetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)

2'-Acetyl-6-methoxypurine arabinoside (hemihydrate)

RN: 121032-43-7 **MP (°C):** 174-176**MW:** 333.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.250E-02	1.083E+01	37	C348	0 0 0 0 0	pH 7.00
5.310E-02	1.770E+01	37	M378	1 2 1 1 2	pH 7.2

3094. C₁₃H₁₆O₄

Diethylacetyl salicylate

Salicylic acid, 2-ethylbutyrate

RN: 100613-21-6 **MP (°C):****MW:** 236.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-03	6.616E-01	25.6	G015	1 0 1 1 2	pH 1.00, pka 4.00, intrinsic

3095. C₁₃H₁₆O₆

Methyl phthalyl ethyl glycolate

RN: **MP (°C):****MW:** 268.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.096E-03	1.099E+00	15	H069	1 0 1 1 1	
1.975E-03	5.297E-01	ns	F014	0 0 0 0 1	

3096. C₁₃H₁₆O₇.0.75H₂O

Helicin (0.75 hydrate)

Salicylaldehyde β-D-glucoside

Benzaldehyde, 2-(β-D-glucopyranosyloxy)-, hydrate (4:3)

RN: 618-65-5 **MP (°C):****MW:** 297.78 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.505E-02	1.639E+01	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3097. C₁₃H₁₇ClO₃

MCPB-ethyl

RN: 10443-70-6 **MP (°C):****MW:** 256.73 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.899E-05	1.001E-02	ns	S460	0 0 0 0 0	

3098. C₁₃H₁₇IN₂O₆

Uridine, 2'-deoxy-5-ido-, 5'-butanoate

5'-Butyryl 5-ido-2'-deoxyuridine

5-Iodo-2'-deoxyuridine 5'-butyrate

RN: 84043-26-5 **MP (°C):** 145.5**MW:** 424.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.450E+03	6.151E+05	25	N332	0 0 0 0 0	pH 7.4

3099. C₁₃H₁₇IN₂O₆

Uridine, 2'-deoxy-5-ido-, 5'-(2-methylpropanoate)

5'-Isobutyryl 5-ido-2'-deoxyuridine

5-Iodo-2'-deoxyuridine 5'-isobutyrate

RN: 84043-27-6 **MP (°C):** 144.5**MW:** 424.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.750E+03	7.423E+05	25	N332	0 0 0 0 0	pH 7.4

3100. C₁₃H₁₇NO

N-Butylcinnamamide

N-Butyl-3-phenyl-2-propenamide

RN: 6299-56-5 **MP (°C):****MW:** 203.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.700E-04	1.972E-01	ns	H350	0 0 0 0 0	

3101. C₁₃H₁₇NO

N,N-Diethylcinnamamide

N,N-Diethyl-3-phenyl-2-propenamide

RN: 3680-04-4 **MP (°C):****MW:** 203.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.450E-03	1.514E+00	ns	H350	0 0 0 0 0	

3102. C₁₃H₁₇NO₃

Acetamide, 2-(benzoyloxy)-*N*-butyl-
RN: 115193-28-7 **MP (°C):** 69.5
MW: 235.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.743E-03	4.100E-01	22	N317	1 1 2 1 2	

3103. C₁₃H₁₇NO₃

N-Acetyl-L-phenylalanine ethyl ester
RN: 2361-96-8 **MP (°C):**
MW: 235.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	2.550E+00	5	L081	2 1 2 2 2	
1.755E-02	4.130E+00	28	L081	2 1 2 2 2	
2.814E-02	6.620E+00	40	L081	2 1 2 2 2	
3.417E-02	8.040E+00	55	L081	2 1 2 2 2	
7.268E-02	1.710E+01	65	L081	2 1 2 2 2	

3104. C₁₃H₁₇NO₃

2-(*p*-Acetaminophenoxy)tetrahydropyran
RN: 51453-65-7 **MP (°C):** 60
MW: 235.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	7.059E-01	ns	H076	0 0 0 0 0	

3105. C₁₃H₁₇NO₃

Pivalyl acetaminophen
Propanoic acid, 2,2-dimethyl-, 4-(acetylamino)phenyl ester
Acetanilide, 4'-hydroxy-, pivalate (ester)
RN: 20675-23-4 **MP (°C):** 162.5–163
MW: 235.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.675E-04	1.100E-01	37	D029	0 0 0 0 0	

3106. C₁₃H₁₇NO₃

Acetamide, 2-(benzoyloxy)-*N*-(1,1-dimethylethyl)-
RN: 106231-52-1 **MP (°C):** 112–113
MW: 235.29 **BP (°C):** 418.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-03	3.200E-01	22	B427	1 0 0 1 1	

3107. C₁₃H₁₇NO₃Acetamide, 2-(benzoyloxy)-*N,N*-diethyl-

RN: 64649-63-4 **MP (°C):** 72.5
MW: 235.29 **BP (°C):** 377.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-03	2.000E+00	22	B427	1 0 0 1 1	
8.500E-03	2.000E+00	22	N317	1 1 2 1 2	in 0.01M HCl

3108. C₁₃H₁₇NO₃Butanamide, 4-(benzoyloxy)-*N,N*-dimethyl-

RN: 115178-78-4 **MP (°C):** 40.5
MW: 235.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.908E-02	1.390E+01	22	N317	1 1 2 1 2	

3109. C₁₃H₁₇NO₄

Benzoic acid, 2-hydroxy-, 2-(diethylamino)-2-oxoethyl ester

N,N-Diethylglycolamide salicylate*N,N*-Diethyl glycolamide salicylate

RN: 65783-69-9 **MP (°C):** 74–75
MW: 251.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.786E-03	7.000E-01	21	B331	1 2 2 1 1	pH 7.4
2.786E-03	7.000E-01	21	B331	0 0 0 0 0	

3110. C₁₃H₁₇NO₄

Butyl acetaminophen

Carbonic acid, butyl ester, ester with 4'-hydroxyacetanilide

Acetanilide, 4'-hydroxy-, butyl carbonate (ester)

RN: 19872-68-5 **MP (°C):** 119.5–120
MW: 251.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.367E-04	1.600E-01	37	D029	0 0 0 0 0	

3111. C₁₃H₁₇NO₄

Isobutyl acetaminophen

Carbonic acid, isobutyl ester, ester with 4'-hydroxyacetanilide

Acetanilide, 4'-hydroxy-, isobutyl carbonate (ester)

RN: 20460-96-2 MP (°C): 119–121

MW: 251.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.512E-03	3.800E-01	37	D029	0 0 0 0 0	

3112. C₁₃H₁₇NO₄*O*-(Pivaloyloxymethyl) salicylamide

RN: MP (°C): 95

MW: 251.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.428E-03	6.100E-01	23	B328	1 2 2 1 1	pH 4

3113. C₁₃H₁₇NO₄

Propanoic acid, 2,2-dimethyl-, [2-(aminocarbonyl)phenoxy]methyl ester

O-Pivaloyloxymethyl salicylamide

RN: 103951-40-2 MP (°C): 94–96

MW: 251.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.428E-03	6.100E-01	23	B328	0 0 0 0 0	

3114. C₁₃H₁₇NO₄Acetamide, 2-(benzoyloxy)-*N*-ethyl-*N*-(2-hydroxyethyl)-

RN: 106231-60-1 MP (°C): 79.5

MW: 251.28 BP (°C): 437.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.298E-02	1.080E+01	22	B427	1 0 0 1 1	in 0.01M HCl
4.298E-02	1.080E+01	22	N317	1 1 2 1 2	

3115. C₁₃H₁₇NO₄*N*-Acetyl-L-tyrosine ethyl esterEthyl *N*-acetyl-L-tyrosinate

RN: 840-97-1 MP (°C):

MW: 251.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.571E-03	1.400E+00	5	L081	2 1 2 2 2	
1.385E-02	3.480E+00	28	L081	2 1 2 2 2	

3116. C₁₃H₁₇NO₅

Acetamide, 2-(benzoyloxy)-N,N-bis(2-hydroxyethyl)-

RN: 106231-61-2 **MP (°C):** 81
MW: 267.28 **BP (°C):** 497.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.694E+00	7.200E+02	22	B427	1 0 0 1 1	
2.694E+00	7.200E+02	22	N317	1 1 2 1 2	in 0.01M HCl

3117. C₁₃H₁₇NO₆

Acetamide, 2-(benzoyloxy)-N-[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-

RN: 115193-31-2 **MP (°C):** 126.5
MW: 283.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.401E-02	1.530E+01	22	N317	1 1 2 1 2	

3118. C₁₃H₁₇N₃O

Aminopyrine

Amidopyrine

4-Dimethylaminoantipyrine

Febrinina

Febron

Itamidone

RN: 58-15-1 **MP (°C):** 108
MW: 231.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.827E-01	6.540E+01	0	C025	0 0 0 0 2	form A
5.607E-01	1.297E+02	4.62	M109	2 1 1 1 0	EFG
5.463E-01	1.264E+02	10.93	M109	2 1 1 1 0	EFG
5.430E-01	1.256E+02	15.02	M109	2 1 1 1 0	EFG
2.291E-01	5.300E+01	20	C025	0 0 0 0 2	form A
5.452E-01	1.261E+02	20.96	M109	2 1 1 1 0	EFG
2.291E-01	5.300E+01	25	P012	0 0 0 0 0	
2.162E-01	5.000E+01	25	P016	1 0 0 1 1	
2.075E-01	4.800E+01	25	P020	2 0 1 1 1	
1.773E+00	4.100E+02	25	P020	2 0 1 1 2	
5.618E-01	1.300E+02	25.35	M109	2 1 1 1 0	EFG
5.965E-01	1.380E+02	29.87	M109	2 1 1 1 0	EFG
2.350E-01	5.436E+01	30	A078	2 1 2 1 0	EFG
2.291E-01	5.300E+01	37	C025	0 0 0 0 2	form A
6.329E-01	1.464E+02	38.37	M109	2 1 1 1 0	EFG
6.646E-01	1.537E+02	49.42	M109	2 1 1 1 0	EFG
3.415E-01	7.900E+01	55	C025	0 0 0 0 2	form A
5.638E-01	1.304E+02	65	C025	0 0 0 0 2	form A
2.162E+00	5.000E+02	69.50	C025	0 0 0 0 2	form A

(continued)

3118. C₁₃H₁₇N₃O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.729E+00	4.000E+02	70	C025	0 0 0 0 2	form B
1.167E+00	2.700E+02	70.50	C025	0 0 0 0 2	form B
2.879E+00	6.660E+02	74.40	C025	0 0 0 0 2	form B
8.647E-01	2.000E+02	77.50	C025	0 0 0 0 2	form B
6.485E-01	1.500E+02	81	C025	0 0 0 0 2	form B
3.243E+00	7.500E+02	84	C025	0 0 0 0 2	form B
3.359E+00	7.770E+02	92	C025	0 0 0 0 2	form B

3119. C₁₃H₁₇N₅O₅

9-(2-O-Propionyl-β-D-arabinofuranosyl)adenine

RN: 65174-99-4 **MP (°C):**
MW: 323.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.618E-04	1.170E-01	37	B306	1 2 0 1 2	pH 7.3

3120. C₁₃H₁₇N₅O₅

9-[5'-(O-Propionyl)-β-D-arabinofuranosyl]adenine ester

RN: 14000-32-9 **MP (°C):** 202.0
MW: 323.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.846E-02	9.200E+00	ns	B134	0 1 1 1 1	

3121. C₁₃H₁₇N₅O₆

9-(1,3-Diacetate-2-propoxymethyl)guanine

RN: 86357-19-9 **MP (°C):** 238
MW: 339.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.709E-03	5.800E-01	25	B360	0 0 0 0 0	

3122. C₁₃H₁₇N₅O₈

9-(1,3-Dimethoxycarbonyl-2-propoxymethyl)guanine

RN: 91625-66-0 **MP (°C):** 178
MW: 371.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.851E-04	1.430E-01	25	B360	0 0 0 0 0	

3123. C₁₃H₁₈ClNO

Monalide

N-(4-Chlorophenyl)-2,2-dimethylvaleramide

RN: 7287-36-7 MP (°C): 87.5

MW: 239.75 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.510E-05	2.280E-02	23	M161	1 0 0 0 2	
9.510E-05	2.280E-02	ns	M061	0 0 0 0 2	

3124. C₁₃H₁₈ClNO

Pentanochlor

Solan

Pentamide, *N*-(3-chloro-4-methylphenyl)-2-methyl-

RN: 2307-68-8 MP (°C): 84

MW: 239.75 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.337E-05	8.000E-03	ns	B185	0 0 0 0 0	
3.545E-05	8.500E-03	rt	M161	0 0 0 0 0	

3125. C₁₃H₁₈CIN₃O₄S₂

Cyclopenthiazide

6-Chloro-3-cyclopentylmethyl-3,4-dihydro-2H-1,2,4-benzothiadiazine-7-sulphonamide 1,1-dioxide

RN: 742-20-1 MP (°C): 235

MW: 379.89 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-04	5.000E-02	rt	A095	0 0 2 2 0	

3126. C₁₃H₁₈Cl₂N₂O₂

Melphalan

4-[bis(2-Chloroethyl)amino]-L-phenylalanine

RN: 148-82-3 MP (°C):

MW: 305.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.442E-02	4.400E+00	30	L343	2 1 1 1 0	
5.561E-03	1.697E+00	ns	S469	0 0 0 0 0	EFG

3127. C₁₃H₁₈N₂O₂

Lenacil

3-Cyclohexyl-5,6-trimethyleneuracil

RN: 2164-08-1 MP (°C): 290

MW: 234.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.561E-05	6.000E-03	25	M061	1 0 0 0 0	
2.561E-05	6.000E-03	25	M161	1 0 0 0 0	

3128. C₁₃H₁₈N₂O₃

Heptabarbital

5-(1-Cyclohepten-1-yl)-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetrione

5-(1-Cyclohepten-1-yl)-5-ethylbarbituric acid

Heptabarbitone

RN: 509-86-4 MP (°C): 174

MW: 250.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.503E-01	25	V033	2 0 1 1 2	
1.000E-03	2.503E-01	25.00	T303	1 0 0 0 1	
1.400E-03	3.504E-01	35.00	T303	1 0 0 0 1	
1.170E-02	2.929E+00	40	N008	1 0 1 1 2	<i>sic</i>
1.800E-03	4.505E-01	45.00	T303	1 0 0 0 1	

3129. C₁₃H₁₈N₂O₃S

Tosylcyclopentylurea

Tosylcyclopentyluree

RN: 1027-87-8 MP (°C):

MW: 282.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.649E-04	7.478E-02	37	A028	1 0 2 1 2	intrinsic
2.650E-04	7.483E-02	37	A046	2 0 1 1 2	

3130. C₁₃H₁₈N₂O₄

Methyl-2-methyl-2-cyclohexenyl-6-methylmalonurate

Methyl 2-methyl-2-cyclohexenyl-6-methylmalonurate

RN: MP (°C): 94

MW: 266.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	5.592E-01	23	B152	1 2 1 1 1	pH 3.5

3131. C₁₃H₁₈N₄O₂S₂

4-Amino-N-(5-pentyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide

Benzenesulfonamide, 4-amino-N-(5-pentyl-1,3,4-thiadiazol-2-yl)-

RN: 71119-30-7 MP (°C):

MW: 326.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.120E-04	3.656E-02	37	A046	2 0 1 1 2	

3132. C₁₃H₁₈N₄O₂S₂

4-Amino-N-(5-isopentyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide

Benzenesulfonamide, 4-amino-N-[5-(3-methylbutyl)-1,3,4-thiadiazol-2-yl]-

RN: 71119-29-4 MP (°C):

MW: 326.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-05	2.938E-02	37	A046	2 0 1 1 2	

3133. C₁₃H₁₈O₂

Ibuprofen

2-(4-Isobutylphenyl)propionic acid

Advil

Ebufac

Rufen

RS-Ibuprofen

RN: 15687-27-1 MP (°C): 75

MW: 206.29 BP (°C): 319.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.320E-04	4.786E-02	4	B411	1 1 1 2 2	
3.340E-05	6.890E-03	5	F306	1 0 1 2 2	intrinsic
1.080E-04	2.228E-02	12	B411	1 1 1 2 2	
1.460E-04	3.012E-02	20	B411	1 1 1 2 2	
7.271E-05	1.500E-02	20	N316	1 0 1 1 0	EFG
3.102E-04	6.400E-02	21	B331	1 2 2 1 2	pH 7.4
2.375E-04	4.900E-02	25	A408	2 0 1 2 0	int
1.018E-04	2.100E-02	25	A427	0 0 0 0 0	
5.478E-05	1.130E-02	25	C314	0 0 0 0 0	
5.560E-05	1.147E-02	25	C314	0 0 0 0 0	
9.430E-04	1.945E-01	25	D345	0 0 0 0 0	
4.300E-05	8.870E-03	25	F301	1 1 0 0 1	pH 2.0, sic
4.300E-05	8.870E-03	25	F306	1 0 1 2 2	intrinsic
5.520E-05	1.139E-02	25	G431	0 0 0 0 0	
2.424E-04	5.000E-02	25	S450	0 0 0 0 0	Intrinsic
2.090E-04	4.311E-02	29	B411	1 1 1 2 2	
7.505E-05	1.548E-02	30	G431	0 0 0 0 0	
1.212E-04	2.500E-02	30	N316	1 0 1 1 0	EFG

(continued)

3133. C₁₃H₁₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.970E-05	2.057E-02	35	G431	0 0 0 0 0	
5.210E-05	1.075E-02	37	F306	1 0 1 2 2	intrinsic
1.551E-04	3.200E-02	37	N316	1 0 1 1 0	EFG
5.332E-05	1.100E-02	37	P432	0 0 0 0 0	
2.909E-04	6.000E-02	37	Y421	0 0 0 0 0	
3.040E-04	6.271E-02	38	B411	1 1 1 2 2	
1.281E-04	2.643E-02	40	G431	0 0 0 0 0	
4.760E-04	9.819E-02	47	B411	1 1 1 2 2	
1.600E-04	3.301E-02	50	M335	1 0 2 1 2	pH 5
2.036E-04	4.200E-02	50	N316	1 0 1 1 0	EFG
2.327E-04	4.800E-02	60	N316	1 0 1 1 0	EFG
2.600E-04	5.363E-02	ns	F327	0 0 1 2 2	
4.848E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.018E-04	2.100E-02	rt	H302	0 0 2 1 2	intrinsic
4.096E-04	8.450E-02	rt	R431	0 0 0 0 0	Average

3134. C₁₃H₁₈O₂

S-Ibuprofen

(S)-(+)-2-(4-Isobutylphenyl)propionic acid

D-Ibuprofen

Seractil

Dexibuprofen

RN: 51146-56-6 MP (°C):

MW: 206.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.320E-04	4.786E-02	4	B411	1 1 1 2 2	
2.560E-04	5.281E-02	12	B411	1 1 1 2 2	
3.390E-04	6.993E-02	20	B411	1 1 1 2 2	
1.790E-03	3.693E-01	25	D345	0 0 0 0 0	
4.670E-04	9.634E-02	29	B411	1 1 1 2 2	
6.090E-04	1.256E-01	38	B411	1 1 1 2 2	

3135. C₁₃H₁₈O₂

r-Ibuprofen

(R)-2-(4-Isobutylphenyl)propanoic acid

r-(−)-p-Isobutylhydratropic acid

l-Ibuprofen

RN: 51146-57-7 MP (°C):

MW: 206.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.790E-03	3.693E-01	25	D345	0 0 0 0 0	

3136. C₁₃H₁₈O₃Hexyl *p*-hydroxybenzoate4-Hydroxybenzoic acid *N*-hexyl ester

RN: 1083-27-8 MP (°C):

MW: 222.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.680E-04	8.180E-02	15	B355	0 0 0 0 0	
3.810E-04	8.469E-02	20	B355	0 0 0 0 0	
6.190E-04	1.376E-01	25	B355	0 0 0 0 0	
1.704E-03	3.789E-01	25	D081	1 2 2 1 2	
3.162E-04	7.029E-02	25	F322	2 0 1 1 0	EFG

3137. C₁₃H₁₈O₃*n*-Hexyl salicylate*n*-Hexyl 2-hydroxybenzoate

RN: 6259-76-3 MP (°C):

MW: 222.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.260E-03	2.800E-01	37	D009	1 2 1 1 1	0.1N HCl

3138. C₁₃H₁₈O₅S

Ethofumesate

2-Ethoxy-2,3-dihydro-3,3-dimethyl-5-benzofuranyl methanesulfonate

Nortran

Tramat

RN: 26225-79-6 MP (°C): 71

MW: 286.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.758E-04	5.034E-02	25	H434	0 0 0 0 0	
3.841E-04	1.100E-01	25	M161	1 0 0 0 2	
3.841E-04	1.100E-01	25	W313	1 0 0 0 1	

3139. C₁₃H₁₈O₇

Salicin

2-(Hydroxymethyl)phenyl-β-D-glucopyranoside

Salicoside

RN: 138-52-3 MP (°C): 199

MW: 286.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-01	4.000E+01	25	F300	1 0 0 0 0	
9.082E-01	2.600E+02	100	F300	1 0 0 0 1	
1.455E-01	4.167E+01	c	D004	0 0 0 0 0	
8.733E-01	2.500E+02	h	D004	0 0 0 0 0	

3140. C₁₃H₁₉NO₂Hexyl *p*-aminobenzoate

4-Aminobenzoic acid hexyl ester

RN: 55791-76-9 MP (°C):

MW: 221.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	2.302E-02	37	F006	1 1 2 2 2	
4.500E-05	9.959E-03	ns	M066	0 0 0 0 1	
4.300E-05	9.516E-03	rt	B016	0 0 1 1 1	pH 7.4

3141. C₁₃H₁₉NO₂

Ibuproxam

2-(4-Isobutylphenyl)propionohydroxamic acid

Ibudros

RN: 53648-05-8 MP (°C): 123

MW: 221.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.037E-04	2.000E-01	ns	M148	0 2 0 0 0	

3142. C₁₃H₁₉NO₄

N,N-Diethyl-6-hydroxynorbornane-2-carboxamide-3,5-lactone

RN: MP (°C):

MW: 253.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.153E-01	2.920E+01	20	K050	1 1 1 1 2	

3143. C₁₃H₁₉NO₄S

Probenecid

Parabenem

4-((Dipropylamino)sulfonyl)benzoic acid

p-(Dipropylsulfamoyl)benzoic

RN: 57-66-9 MP (°C): 195

MW: 285.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.262E-05	3.600E-03	22.5	B422	2 0 2 2 2	
2.089E-06	5.962E-04	ns	R427	0 0 0 0 0	

3144. C₁₃H₁₉N₃O₄

N-(1-Ethylpropyl)-2,6-dinitro-3,4-xylidine

Pendimethalin

RN: 40487-42-1 **MP (°C):** 56.5
MW: 281.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.066E-06	3.000E-04	20	M161	1 0 0 0 0	
1.081E-03	3.040E-01	ns	B185	0 0 0 0 0	
1.066E-06	3.000E-04	ns	V414	0 0 0 0 0	

3145. C₁₃H₁₉N₃O₆S

Nitralin

4-(Methylsulfonyl)-2,6-dinitro-N,N-dipropylaniline

RN: 4726-14-1 **MP (°C):** 151
MW: 345.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-06	6.000E-04	22	M161	1 0 0 0 0	
1.737E-06	6.000E-04	25	B200	1 0 0 0 0	
1.737E-07	6.000E-05	25	P028	0 0 0 0 0	
1.737E-06	6.000E-04	ns	M061	0 0 0 0 0	

3146. C₁₃H₂₀N₂O

Prilocaine

RN: 721-50-6 **MP (°C):**
MW: 220.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-02	6.169E+00	25	D402	1 2 2 2 0	EFG
2.900E-02	6.389E+00	37	D402	1 2 2 2 0	EFG

3147. C₁₃H₂₀N₂O₂

Procaine

Novacaine

Novokain

RN: 59-46-1 **MP (°C):** 60
MW: 236.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-02	9.453E+00	30	L068	1 0 0 1 0	EFG
4.200E-02	9.925E+00	37.5	L034	2 2 0 1 2	pH 7.4
5.494E-03	1.298E+00	ns	E031	0 0 2 1 2	
2.700E-02	6.381E+00	ns	M066	0 0 0 0 1	

3148. C₁₃H₂₀N₂O₂N,N'-Diethyl-bicyclo(2.2.1)hept-5-ene-2,3-*trans*-dicarboxamide

RN: MP (°C):
MW: 236.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.216E-02	7.600E+00	20	K050	1 1 1 1 2	

3149. C₁₃H₂₀N₂O₂

4-Aminobenzoic acid-2-(butyl-amino)ethyl ester

2-(Butylamino)ethyl 4-aminobenzoate

RN: MP (°C):
MW: 236.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-04	4.017E-02	ns	M066	0 0 0 0 1	

3150. C₁₃H₂₀N₂O₃

5-Allyl-5-ethylbutylbarbituric acid

RN: MP (°C):
MW: 252.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.587E-02	4.004E+00	20	J030	1 2 2 2 2	
2.579E-02	6.507E+00	37	J030	1 2 2 2 2	

3151. C₁₃H₂₀N₂O₃

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-(1,1-dimethylethyl)-5-(3-methyl-2-butenyl)

5-*t*-Butyl-5-(3-methylbut-2-enyl)barbiturate

RN: 143585-02-8 MP (°C):
MW: 252.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-04	7.090E-02	25	P350	0 0 0 0 0	intrinsic

3152. C₁₃H₂₀O

2-Hexyl-6-methylphenol

o-Cresol, 6-hexyl-

RN: 106593-25-3 MP (°C):
MW: 192.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	5.000E-03	25	L020	1 0 0 0 0	

3153. C₁₃H₂₀O

2-Hexyl-4-methylphenol

2-Hexyl-*p*-cresol

RN: 54612-53-2 **MP (°C):**
MW: 192.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.467E-05	6.667E-03	25	L020	1 0 0 0 0	

3154. C₁₃H₂₀O*b*-Damascone*b*-Damascone, *trans*-*trans*-2,6,6-Trimethyl-1-crotonylcyclohex-1-ene*trans*-*b*-DamasconeDamascone β

RN: 23726-91-2 **MP (°C):**
MW: 192.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.923E-01	25	D407	1 0 2 2 2	

3155. C₁₃H₂₀O β -Damascone

4-(2,6,6-Trimethyl cyclohex-1-enyl)but-2-en-4-one

Damasione

RN: 23726-92-3 **MP (°C):**
MW: 192.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	1.923E-01	ns	S460	0 0 0 0 0	

3156. C₁₃H₂₀O*o*-*n*-Heptylphenol*2*-*n*-Heptylphenol

RN: 5284-22-0 **MP (°C):**
MW: 192.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.118E-05	1.176E-02	25	L022	1 0 0 0 0	

3157. C₁₃H₂₀O

4-Hexyl-2-methylphenol

o-Cresol, 4-hexyl-

RN: 3280-61-3 **MP (°C):**
MW: 192.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	5.000E-03	25	L020	1 0 0 0 0	

3158. C₁₃H₂₀O

α-Ionone

α-Irisone

Cyclocitrylideneacetone

Ionone α

Buten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-

RN: 127-41-3 **MP (°C):**
MW: 192.30 **BP (°C):** 229

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.508E-04	1.059E-01	ns	S460	0 0 0 0 0	

3159. C₁₃H₂₀O*p*-*n*-Heptylphenol4-*n*-Heptylphenol

RN: 1987-50-4 **MP (°C):**
MW: 192.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.778E-05	1.111E-02	25	L022	1 0 0 0 0	

3160. C₁₃H₂₁NO₃

Salbutamol

Albuterol

Ventolin

RN: 18559-94-9 **MP (°C):** 151
MW: 239.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-02	1.771E+01	20	M380	1 0 2 1 0	EFG
7.500E-02	1.795E+01	25	M380	1 0 2 1 0	EFG
7.400E-02	1.771E+01	37	M380	1 0 2 1 0	EFG
5.885E-02	1.408E+01	ns	A092	0 0 0 0 0	

3161. C₁₃H₂₁O₃PSS-Benzyl *O,O*-di-isopropyl phosphorothioate

Isokitazine

Kitazin P

IBP

Iprobenfos

Kitazin L

RN: 26087-47-8 MP (°C):

MW: 288.35 BP (°C): 126

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.468E-03	1.000E+00	18	M161	1 0 0 0 0	

3162. C₁₃H₂₁O₄PS

4-(Methylthio)phenyl dipropyl phosphate

O,O-Dipropyl *O*-4-methylthiophenyl phosphate

Propaphos

Kayaphos

Kayphosnac

RN: 7292-16-2 MP (°C):

MW: 304.35 BP (°C): 176

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.107E-04	1.250E-01	25	M161	1 0 0 0 2	

3163. C₁₃H₂₂NO₃PS

Fenamiphos

1-(Methylethyl)-*O*-ethyl-*O*-(3-methyl-4-(methylthio)phenyl)phosphoramidate

Nemacur

Bay 68138

RN: 22224-92-6 MP (°C):

MW: 303.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.008E-03	3.059E-01	10	B324	0 0 0 0 0	
1.009E-03	3.061E-01	10	B324	0 0 0 0 0	
2.291E-03	6.950E-01	20	B179	0 0 0 0 0	
1.084E-03	3.288E-01	20	B300	2 1 1 1 2	
1.085E-03	3.291E-01	20	B324	0 0 0 0 0	
1.084E-03	3.289E-01	20	B324	0 0 0 0 0	
1.381E-03	4.189E-01	30	B324	0 0 0 0 0	
1.381E-03	4.188E-01	30	B324	0 0 0 0 0	
2.307E-03	7.000E-01	rt	M161	0 0 0 0 2	

3164. C₁₃H₂₂N₂O

Isonoruron

Urea, 3-[hexahydro-4,7-methanoindan-1(or 2)-yl]-1,1-dimethyl-

Tricuron

BAS 2103H

RN: 28346-65-8 MP (°C): 165

MW: 222.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.895E-04	2.200E-01	20	M161	1 0 0 0 2	

3165. C₁₃H₂₂N₂O

Noruron

3-(Hexahydro-4,7-methanoindan-5-yl)-1,1-dimethylurea

Norea

RN: 18530-56-8 MP (°C): 171

MW: 222.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.747E-04	1.500E-01	20	M061	1 0 0 0 2	
6.747E-04	1.500E-01	25	B200	1 0 0 0 2	
6.747E-04	1.500E-01	ns	G036	0 0 0 0 2	

3166. C₁₃H₂₂N₂O₃5-Ethyl-5-*n*-heptylbarbituric acid

5-Ethyl-5-heptylbarbituric acid

5-Ethyl-5-heptylbarbiturate

RN: 60784-70-5 MP (°C):

MW: 254.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.050E-04	1.539E-01	25	M310	2 2 2 2 2	

3167. C₁₃H₂₂O₃

Methyl dihydrojasmonate

Hedione

Methyl 3-oxo-2-pentylcyclopentaneacetate

Claigeon

RN: 24851-98-7 MP (°C):

MW: 226.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.767E-03	3.998E-01	25	M350	1 0 1 1 1	

3168. C₁₃H₂₄N₃O₃PS

Pirimiphos-ethyl

Diethyl *O*-(2-(diethylamino)-6-methyl-4-pyrimidinyl) phosphorothioate

Fernex

Primotec

Solgard

RN: 23505-41-1 **MP (°C):**
MW: 333.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-05	3.967E-03	20	B300	2 1 1 1 2	
<3.00E-06	<1.00E-03	30	M161	1 0 0 0 0	

3169. C₁₃H₂₄N₄O₃S

Bupirimate

5-Butyl-2-(ethylamino)-6-methyl-4-pyrimidinyl dimethylsulfamate

Nimrod

RN: 41483-43-6 **MP (°C):** 50.5
MW: 316.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.918E-05	2.189E-02	ns	R427	0 0 0 0 0	
6.953E-05	2.200E-02	rt	M161	0 0 0 0 1	

3170. C₁₃H₂₄N₆1-(Hexamethyleneiminel)-3,5-bis(dimethylamino)-*s*-triazine1,3,5-Triazine-2,4-diamine, 6-(hexahydro-1H-azepin-1-yl)-*N,N,N',N'*-tetramethyl-

RN: 125867-92-7 **MP (°C):**
MW: 264.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.265E-05	5.988E-03	25	B386	0 0 0 0 0	

3171. C₁₃H₂₄O₄Octyl α -acetoxypropionate

Propanoic acid, 2-(acetoxy)-, octyl ester

RN: 6283-90-5 **MP (°C):**
MW: 244.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.093E-04	1.000E-01	25	R006	2 2 0 1 1	

3172. C₁₃H₂₄O₄

1,11-Undecanedicarboxylic acid

1,13-Tridecanedioic acid

Brassylic acid

RN: 505-52-2**MP (°C):** 111**MW:** 244.33**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.139E-03	1.500E+00	21	B040	1 0 1 1 1	<i>sic</i>
1.637E-04	4.000E-02	24	F300	1 0 0 0 0	<i>sic</i>

3173. C₁₃H₂₅NO₃

Dibutylaceturethane

RN: MP (°C):**MW:** 243.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.287E-04	7.999E-02	44	O021	1 2 0 0 0	

3174. C₁₃H₂₆N₂O₂

N,N,N',N'-Tetramethylazelamide

Nonanediamide, N,N,N',N'-tetramethyl-

RN: 13424-87-8 **MP (°C):****MW:** 242.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E+00	9.452E+02	30	D010	1 2 1 1 2	

3175. C₁₃H₂₆O₂

n-Tridecanoic acid

Tridecanoic acid

RN: 638-53-9 **MP (°C):** 41.5**MW:** 214.35 **BP (°C):** 236

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.797E-05	2.100E-02	0	B136	1 0 2 1 1	
1.540E-04	3.300E-02	20	B136	1 0 2 1 1	
1.539E-04	3.300E-02	20.0	R001	1 1 1 1 1	
1.773E-04	3.800E-02	30	B136	1 0 2 1 1	
1.773E-04	3.800E-02	30.0	R001	1 1 1 1 1	
2.053E-04	4.400E-02	45	B136	1 0 2 1 1	
2.053E-04	4.400E-02	45.0	R001	1 1 1 1 1	
2.519E-04	5.400E-02	60	B136	1 0 2 1 1	
2.519E-04	5.400E-02	60.0	R001	1 1 1 1 1	
9.797E-05	2.100E-02	.0	R001	1 1 1 1 1	

3176. C₁₃H₂₆O₂

Methyl laurate

Dodecanoic acid methyl ester

Methyl dodecanoate

RN: 111-82-0**MP (°C):** 41**MW:** 214.35**BP (°C):** 261

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.05E-05	<4.40E-03	20	M337	2 1 2 2 1	

3177. C₁₃H₂₆O₃*n*-Octyl β-ethoxypropionate**RN:** 111-82-0**MP (°C):****MW:** 230.35**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.34E-04	<10.00E-02	25	D002	1 2 1 1 0	

3178. C₁₃H₂₆O₃

Decyl lactate

2-Hydroxypropionic acid decyl ester

RN: 42175-34-8**MP (°C):****MW:** 230.35**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.682E-04	2.000E-01	25	R006	2 2 0 1 0	

3179. C₁₃H₂₆O₄

1,3-Dioxolane-4-methanol, 2-[2-(hexyloxy)ethyl]-2-methyl

RN: 124485-63-8**MP (°C):****MW:** 246.35**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-02	3.942E+00	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

3180. C₁₃H₂₈

Tridecane

RN: 629-50-5**MP (°C):** -5.5**MW:** 184.37**BP (°C):** 235.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.170E-09	4.000E-07	25	T423	0 0 0 0 0	

3181. C₁₄H₄N₂O₂S₂

Dithianon

1,4-Dithiaanthraquinone-2,3-dinitrile

2,3-Dicyano-1,4-dithiaanthraquinone

RN: 3347-22-6 **MP (°C):** 225**MW:** 296.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.687E-06	5.000E-04	ns	A305	0 0 0 0 0	
4.677E-07	1.386E-04	ns	R427	0 0 0 0 0	

3182. C₁₄H₆Cl₂F₄N₂O₂

Teflubenzuron

Nomolt

RN: 83121-18-0 **MP (°C):****MW:** 381.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.466E-08	9.400E-06	20	M402	0 0 0 0 0	

3183. C₁₄H₆N₂O₄

1,4,5,8-Naphthalenediimide

1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide

1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide

1,4,5,8-Naphthalenetetracarboxylic acid diimide

1,4,5,8-Naphthalenetetracarboxylic diimide

Benzo[Imn][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone

RN: 5690-24-4 **MP (°C):****MW:** 266.21 **BP (°C):** 656.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		23	B410	2 1 2 2 2	

3184. C₁₄H₆O₈

Ellagic acid

2,3,7,8-Tetrahydroxy(1)benzopyrano(5,4,3-cde)(1)benzopyran-5,10-dione

Elagostasin

Benzoaric acid

Alizarine yellow

4,4',5,5',6,6'-Hexahydrodiphenic acid 2,6,2',6'-dilactone

RN: 476-66-4 **MP (°C):** >360**MW:** 302.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.210E-05	9.700E-03	37	B438	0 0 0 0 0	

3185. C₁₄H₇ClO₅S

1,5-Chloroanthraquinone sulfonic acid

1-Anthracenesulfonic acid, 5-chloro-9,10-dihydro-9,10-dioxo-

RN: MP (°C):

MW: 322.73 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.033E+00	3.333E+02	18	F047	1 2 1 1 0	

3186. C₁₄H₇ClO₅S

1,7-Chloroanthraquinone sulfonic acid

RN: MP (°C):

MW: 322.73 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-01	2.000E+02	18	F047	1 2 1 1 0	

3187. C₁₄H₇ClO₅S

1,6-Chloroanthraquinone sulfonic acid

2-Anthracenesulfonic acid, 5-chloro-9,10-dihydro-9,10-dioxo-

RN: 300360-23-0 MP (°C):

MW: 322.73 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.197E-01	2.000E+02	18	F047	1 2 1 1 0	

3188. C₁₄H₈Cl₂N₄

Clofentezine

3,6-bis(2-Chlorophenyl)-1,2,4,5-tetrazine

Apollo

Acaristop

bis(2-Chlorophenyl)-1,2,4,5-tetrazine

Panatac

RN: 74115-24-5 MP (°C): 182.3

MW: 303.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-09	2.522E-06	ns	R424	0 0 0 0 0	
8.318E-09	2.522E-06	ns	R427	0 0 0 0 0	

3189. C₁₄H₈Cl₄

2,4'-Dichlorodiphenyldichloroethylene

1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethylene

o,p'-DDE**RN:** 3424-82-6 **MP (°C):** 76.5**MW:** 318.03 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.402E-07	1.400E-04	25	B083	2 2 1 2 2	particle size 5 µm

3190. C₁₄H₈Cl₄*p,p'*-Dichlorodiphenyldichloroethylene

2,2-bis(4-Chlorophenyl)-1,1-dichloroethylene

p,p'-DDE**RN:** 72-55-9 **MP (°C):** 89.0**MW:** 318.03 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.729E-07	5.500E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.258E-07	4.000E-05	20	C053	0 0 0 0 0	
1.258E-07	4.000E-05	20	F071	1 1 2 1 1	
3.773E-07	1.200E-04	25	B083	2 2 1 2 2	particle size 5 µm
3.773E-07	1.200E-04	25	I308	0 0 0 0 0	
4.088E-09	1.300E-06	25	M134	1 2 1 1 1	
4.402E-08	1.400E-05	25	W025	1 0 1 1 1	
7.389E-07	2.350E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.415E-06	4.500E-04	45	B083	2 2 1 2 2	particle size 5 µm
4.717E-09	1.500E-06	ns	M110	0 0 0 0 0	EFG
4.088E-09	1.300E-06	ns	M118	0 1 1 1 1	

3191. C₁₄H₈O₂

Anthraquinone

9,10-Anthaquinone

9,10-Dioxoanthracene

Corbit

Morkit

Hoelite

RN: 84-65-1 **MP (°C):** 286**MW:** 208.22 **BP (°C):** 377

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-06	1.353E-03	25	E014	2 2 2 1 1	pH 7.3
3.000E-06	6.247E-04	ns	G077	0 0 0 0 1	

3192. C₁₄H₈O₄

Alizarin

Alizarine

C.I. Mordant red 11

RN: 72-48-0

MP (°C): 290

MW: 240.22

BP (°C): 430

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-05	3.123E-03	25	B333	0 0 0 0 0	<i>sic</i>
1.664E-03	3.998E-01	rt	D021	0 0 1 1 1	<i>sic</i>

3193. C₁₄H₈O₄

Quinizarin

1,4-Dihydroxyanthraquinone

C.I. Pigment violet 12

RN: 81-64-1

MP (°C): 192

MW: 240.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-07	9.609E-05	25	B333	0 0 0 0 0	
6.000E-05	1.441E-02	98.59	M180	0 0 2 2 0	EFG
9.200E-05	2.210E-02	111.46	M180	0 0 2 2 0	EFG
1.100E-04	2.642E-02	117.47	M180	0 0 2 2 0	EFG
1.800E-04	4.324E-02	123.67	M180	0 0 2 2 0	EFG
2.000E-04	4.804E-02	126.84	M180	0 0 2 2 0	EFG
2.100E-04	5.045E-02	135.00	M180	0 0 2 2 0	EFG
4.900E-04	1.177E-01	141.78	M180	0 0 2 2 0	EFG
7.500E-04	1.802E-01	152.37	M180	0 0 2 2 0	EFG

3194. C₁₄H₈O₅

Purpurin

1,2,4-Trihydroxy-anthrachinon

RN: 81-54-9

MP (°C):

MW: 256.22

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	6.405E-03	25	B333	0 0 0 0 0	

3195. C₁₄H₈O₆

Quinalizarin

1,2,5,8-Tetrahydroxyanthraquinone

9,10-Anthracenedione

Alizarine Bordeaux B

Mordant violet 26

RN: 81-61-8 **MP (°C):****MW:** 272.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-06	2.586E-03	25	B333	0 0 0 0 0	

3196. C₁₄H₈O₈S₂

Anthraquinone-1,8-disulfonic acid

1,8-Disulfonic acid anthraquinone

Anthracchinon-disulfosaeure-(1,8)

1,8-Anthaquinone disulfonic acid

RN: 82-48-4 **MP (°C):** 293**MW:** 368.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E+00	4.000E+02	18	F047	1 2 1 1 1	

3197. C₁₄H₈O₈S₂

1,6-Anthaquinone disulfonic acid

Anthraquinone-1,6-disulfonic acid

RN: 14486-58-9 **MP (°C):** 216**MW:** 368.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.357E+00	5.000E+02	18	F047	1 2 1 1 0	

3198. C₁₄H₈O₈S₂

1,5-Anthaquinone disulfonic acid

Anthraquinone-1,5-disulfonic acid

RN: 252967-17-2 **MP (°C):** 310.0**MW:** 368.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.086E+00	4.000E+02	18	F047	1 2 1 1 1	

3199. C₁₄H₉ClF₂N₂O₂

Difluron

Diflubenzuron

TH 6040

RN: 35367-38-5 **MP (°C):** 239**MW:** 310.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.437E-07	2.000E-04	20	M161	1 0 0 0 0	
2.865E-07	8.900E-05	20	M402	0 0 0 0 0	
6.437E-07	2.000E-04	20	R303	1 0 0 0 0	
9.656E-07	3.000E-04	24	C105	2 1 2 2 2	
1.609E-06	5.000E-04	ns	M110	0 0 0 0 0	EFG
2.570E-07	7.986E-05	ns	R427	0 0 0 0 0	

3200. C₁₄H₉ClF₃NO₂

Efavirenz

8-Chloro-5-(2-cyclopropylethynyl)-5-(trifluoromethyl)-4-oxa-2-azabicyclo [4.4.0]deca-7,9,11-trien-3-one

RN: 154598-52-4 **MP (°C):****MW:** 315.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-05	8.000E-03	ns	A426	0 0 0 0 0	intrinsic
3.168E-05	1.000E-02	ns	K444	0 0 0 0 0	

3201. C₁₄H₉Cl₂NO₅

Bifenox

5-(2,4-Dichlorphenoxy)-2-nitro-benzoic acid methyl ester

Modown 4 flowable

Modown

RN: 42576-02-3 **MP (°C):** 85**MW:** 342.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.461E-06	5.000E-04	ns	M110	0 0 0 0 0	EFG
1.023E-06	3.500E-04	ns	M161	0 0 0 0 1	
1.023E-06	3.501E-04	ns	R427	0 0 0 0 0	

3202. C₁₄H₉Cl₅*o,p'*-DDT

1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2,2-trichloroethane

2,4'-DDT

2-(2-Chlorophenyl)-2-(4-chlorophenyl)-1,1,1-trichloroethane

RN: 789-02-6 **MP (°C):** 74.0**MW:** 354.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.410E-07	5.000E-05	15	B083	2 2 1 2 1	particle size 5 μm
2.398E-07	8.500E-05	25	B083	2 2 1 2 1	particle size 5 μm
2.398E-07	8.500E-05	25	I308	0 0 0 0 0	
7.334E-08	2.600E-05	25	W025	1 0 2 2 1	
3.808E-07	1.350E-04	35	B083	2 2 1 2 2	particle size 5 μm
5.642E-07	2.000E-04	45	B083	2 2 1 2 2	particle size 5 μm

3203. C₁₄H₉Cl₅*p,p'*-DDT2,2-bis(*p*-Chlorophenyl)-1,1,1-trichloroethane*p,p'*-TDEE**RN:** 50-29-3 **MP (°C):** 108.5**MW:** 354.49 **BP (°C):** 260

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.385E-09	1.200E-06	0	G319	0 0 0 0 0	
1.664E-08	5.900E-06	2	B186	2 0 2 2 2	
4.796E-08	1.700E-05	15	B083	2 2 1 2 1	particle size 5 μm
1.834E-07	6.500E-05	15	B083	2 2 1 2 1	particle size 5 μm
2.800E-07	9.926E-05	18	G054	1 0 1 0 1	
1.410E-08	5.000E-06	20	C111	1 0 0 0 0	
1.410E-08	5.000E-06	20	C113	1 0 2 1 1	
1.128E-07	4.000E-05	20	E048	1 2 1 1 0	
2.172E-08	7.700E-06	20	F303	1 2 1 2 1	
2.172E-08	7.700E-06	20	W319	1 2 1 2 1	
1.552E-08	5.500E-06	24	C311	0 0 0 0 0	EFG
1.523E-08	5.400E-06	24	C313	0 0 0 0 0	
2.821E-09	1.000E-06	24	K069	2 0 0 1 1	
7.079E-08	2.510E-05	24.99	K436	0 0 0 0 0	
3.385E-09	1.200E-06	25	B036	1 1 0 1 1	
3.949E-07	1.400E-04	25	B083	2 2 1 2 2	particle size 5 μm
7.052E-08	2.500E-05	25	B083	2 2 1 2 1	particle size 5 μm
4.796E-09	1.700E-06	25	B093	2 2 2 2 1	
1.055E-07	3.740E-05	25	B186	2 0 2 2 2	
9.168E-09	3.250E-06	25	F071	1 1 2 1 1	
3.385E-09	1.200E-06	25	M040	1 0 0 1 1	
3.385E-09	1.200E-06	25	M130	1 0 0 0 1	
2.821E-09	1.000E-06	25	P085	0 0 0 0 0	
1.552E-08	5.500E-06	25	W025	1 0 2 2 1	
3.385E-09	1.200E-06	26.70	L095	2 2 1 1 2	

(continued)

3203. C₁₄H₉Cl₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-07	3.700E-05	35	B083	2 2 1 2 1	particle size 5 µm
7.334E-07	2.600E-04	35	B083	2 2 1 2 2	particle size 5 µm
1.269E-07	4.500E-05	37.50	B186	2 0 2 2 2	
1.269E-07	4.500E-05	45	B083	2 2 1 2 1	particle size 5 µm
1.439E-06	5.100E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.552E-08	5.500E-06	ns	C318	0 0 0 0 0	
3.385E-09	1.200E-06	ns	I300	0 0 0 0 1	
4.796E-09	1.700E-06	ns	K138	0 0 0 0 2	
2.821E-09	1.000E-06	ns	M061	0 0 0 0 0	
3.103E-09	1.100E-06	ns	M110	0 0 0 0 0	EFG
5.642E-09	2.000E-06	ns	M138	0 0 0 0 0	
8.745E-09	3.100E-06	ns	M344	0 0 0 0 1	
2.821E-08	1.000E-05	ns	V414	0 0 0 0 0	
2.539E-07	9.000E-05	ns	V414	0 0 0 0 0	

3204. C₁₄H₉Cl₅O

Dicofol

4-Chloro-α-(4-chlorophenyl)-α-(trichloromethyl)benzenemethanol

4,4'-Dichloro-α-(trichloromethyl)benzhydrol

Acarin

Carbox

Cekudifol

RN: 115-32-2 MP (°C): 79

MW: 370.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.563E-06	1.320E-03	25	W025	1 0 2 2 2	

3205. C₁₄H₉F

1-Fluoroanthracene

RN: 7651-80-1 MP (°C):

MW: 196.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E-06	2.600E-04	ns	M344	0 0 0 0 2	

3206. C₁₄H₉NO₂

2-Aminoanthraquinone

2-Amino-9,10-anthracenedione

2-Amino-9,10-anthraquinone

Aminoanthraquinone

AAQ

RN: 117-79-3 **MP (°C):** 310
MW: 223.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.300E-07	1.630E-04	25	B333	0 0 0 0 0	

3207. C₁₄H₉NO₂

1-Aminoanthraquinone

1-Amino-9,10-anthracenedione

1-Amino-9,10-anthraquinone

RN: 82-45-1 **MP (°C):** 254
MW: 223.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	3.125E-04	25	B333	0 0 0 0 0	

3208. C₁₄H₉NO₂

2-Phenyl-3,1-benzoxazin-4-one

Bentranil

Linarotox

Linurotox

RN: 1022-46-4 **MP (°C):** 123.5
MW: 223.23 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.464E-05	5.500E-03	20	M161	1 0 0 0 0	

3209. C₁₄H₉NO₂S

4-Benzoyl phenylisothiocyanate

4-Isothiocyanatobenzophenone

RN: 26328-59-6 **MP (°C):**
MW: 255.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-05	3.574E-03	25	K032	2 2 0 1 1	

3210. C₁₄H₉NO₃

1-Amino-4-hydroxyanthraquinone

C.I. Disperse red 15

Disperse red 15

Celliton fast pink B

RN: 116-85-8

MP (°C): 208

MW: 239.23

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-06	2.871E-04	25	B333	0 0 0 0 0	
1.129E-05	2.700E-03	60	P313	0 0 0 0 0	average of 2
1.797E-05	4.300E-03	70	P313	0 0 0 0 0	average of 2
2.320E-05	5.550E-03	80	P313	0 0 0 0 0	average of 2
4.828E-05	1.155E-02	90	P313	0 0 0 0 0	average of 2
1.500E-04	3.588E-02	98.59	M180	0 0 2 2 0	EFG
2.500E-04	5.981E-02	111.46	M180	0 0 2 2 0	EFG
3.000E-04	7.177E-02	114.44	M180	0 0 2 2 0	EFG
4.500E-04	1.077E-01	122.10	M180	0 0 2 2 0	EFG
6.000E-04	1.435E-01	126.84	M180	0 0 2 2 0	EFG
6.500E-04	1.555E-01	130.07	M180	0 0 2 2 0	EFG
1.500E-03	3.588E-01	152.37	M180	0 0 2 2 0	EFG

3211. C₁₄H₁₀

Phenanthrene

Phenanthracene

RN: 85-01-8

MP (°C): 100

MW: 178.24

BP (°C): 340

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.462E-06	2.607E-04	- .7	N053	1 0 0 1 0	
1.970E-06	3.511E-04	4.00	M082	1 1 1 2 2	
1.970E-06	3.511E-04	4.00	M151	2 1 2 2 2	
2.027E-06	3.613E-04	4.04	M183	1 2 1 1 2	
2.265E-06	4.037E-04	4.62	N053	1 0 0 1 0	EFG
2.373E-06	4.230E-04	8.50	M063	2 1 2 2 2	
2.370E-06	4.224E-04	8.50	M082	1 1 1 2 2	
2.370E-06	4.224E-04	8.50	M151	2 1 2 2 2	
2.375E-06	4.233E-04	8.54	M183	1 2 1 1 2	
2.626E-06	4.680E-04	10.00	M063	2 1 2 2 2	
2.630E-06	4.688E-04	10.00	M082	1 1 1 2 2	
2.630E-06	4.688E-04	10.00	M151	2 1 2 2 2	
2.628E-06	4.684E-04	10.04	M183	1 2 1 1 2	
3.055E-06	5.446E-04	10.13	N053	1 0 0 1 0	EFG
2.873E-06	5.120E-04	12.50	M063	2 1 2 2 2	
2.870E-06	5.115E-04	12.50	M082	1 1 1 2 2	
2.870E-06	5.115E-04	12.50	M151	2 1 2 2 2	
2.875E-06	5.124E-04	12.54	M183	1 2 1 1 2	
3.759E-06	6.700E-04	14.20	N053	1 0 0 1 0	EFG
3.372E-06	6.010E-04	15.00	M063	2 1 2 2 2	

(continued)

3211. C₁₄H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.370E-06	6.007E-04	15.00	M082	1 1 1 2 2	
3.370E-06	6.007E-04	15.00	M151	2 1 2 2 2	
3.375E-06	6.015E-04	15.04	M183	1 2 1 1 2	
1.500E-05	2.674E-03	20	E025	1 0 2 2 2	
6.200E-06	1.105E-03	20	H306	1 0 1 2 1	
5.061E-06	9.020E-04	20	V416	0 0 0 0 0	
4.420E-06	7.878E-04	20.00	M082	1 1 1 2 2	
4.420E-06	7.878E-04	20.00	M151	2 1 2 2 2	
4.419E-06	7.877E-04	20.04	M183	1 2 1 1 2	
4.578E-06	8.160E-04	21.00	M063	2 1 2 2 2	
4.580E-06	8.163E-04	21.00	M082	1 1 1 2 2	
4.580E-06	8.163E-04	21.00	M151	2 1 2 2 2	
4.582E-06	8.167E-04	21.04	M183	1 2 1 1 2	
7.200E-06	1.283E-03	22	A413	2 0 2 2 1	
5.582E-06	9.950E-04	24.30	M063	2 1 2 2 2	
5.360E-06	9.553E-04	24.30	M082	1 1 1 2 2	
5.360E-06	9.553E-04	24.30	M151	2 1 2 2 2	
5.363E-06	9.558E-04	24.34	M183	1 2 1 1 2	
6.284E-06	1.120E-03	24.60	W003	2 2 2 2 2	average of 2
5.577E-06	9.940E-04	25	A001	1 2 2 2 2	
6.059E-06	1.080E-03	25	B319	2 0 1 2 1	
4.617E-06	8.230E-04	25	D406	1 2 2 2 2	
6.003E-06	1.070E-03	25	E004	2 1 2 2 2	
9.000E-06	1.604E-03	25	K001	2 2 2 2 0	
5.611E-06	1.000E-03	25	L332	1 1 1 1 1	
7.238E-06	1.290E-03	25	M064	1 1 2 2 2	
6.620E-06	1.180E-03	25	M342	1 0 1 1 2	
3.815E-06	6.800E-04	25	P340	0 0 0 0 0	
7.278E-06	1.297E-03	25	T066	1 0 0 0 2	
5.610E-06	9.999E-04	25	W300	2 2 2 2 2	
5.622E-06	1.002E-03	25.00	M151	2 1 1 2 2	
6.800E-06	1.212E-03	25.04	V013	2 2 2 2 2	
5.690E-06	1.014E-03	25.35	N053	1 0 0 1 0	EFG
8.977E-06	1.600E-03	27	D003	1 0 0 1 1	
9.257E-06	1.650E-03	27	D043	2 0 0 0 2	average of 2
7.854E-06	1.400E-03	28.95	N053	1 0 0 1 0	EFG
6.845E-06	1.220E-03	29	M071	2 2 2 2 2	
6.845E-06	1.220E-03	29.00	M151	2 1 1 2 2	
7.165E-06	1.277E-03	29.90	M063	2 1 2 2 2	
7.160E-06	1.276E-03	29.90	M082	1 1 1 2 2	
7.160E-06	1.276E-03	29.90	M151	2 1 2 2 2	
8.360E-06	1.490E-03	29.90	W003	2 2 2 2 2	
6.867E-06	1.224E-03	29.94	M183	1 2 1 1 2	
8.304E-06	1.480E-03	30.30	W003	2 2 2 2 2	average of 2
1.035E-05	1.845E-03	34.53	N053	1 0 0 1 0	EFG
1.375E-05	2.450E-03	38.40	W003	2 2 2 2 2	average of 2
1.440E-05	2.566E-03	40	V416	0 0 0 0 0	
1.274E-05	2.270E-03	40.10	W003	2 2 2 2 2	average of 3
2.171E-05	3.870E-03	47.50	W003	2 2 2 2 2	average of 3 <i>(continued)</i>

3211. C₁₄H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.429E-05	4.330E-03	50.10	W003	2 2 2 2 2	average of 3
2.289E-05	4.080E-03	50.20	W003	2 2 2 2 2	average of 3
3.164E-05	5.640E-03	54.70	W003	2 2 2 2 2	average of 3
4.034E-05	7.190E-03	59.20	W003	2 2 2 2 2	average of 3
3.559E-05	6.344E-03	60	V416	0 0 0 0 0	
4.096E-05	7.300E-03	60.50	W003	2 2 2 2 1	average of 3
5.498E-05	9.800E-03	65.10	W003	2 2 2 2 1	average of 3
7.013E-05	1.250E-02	70.70	W003	2 2 2 2 2	average of 3
7.238E-05	1.290E-02	71.90	W003	2 2 2 2 2	
8.528E-05	1.520E-02	73.40	W003	2 2 2 2 2	
7.238E-06	1.290E-03	ns	H123	0 0 0 0 0	
7.238E-06	1.290E-03	ns	K304	0 0 0 0 2	
7.238E-06	1.290E-03	ns	M344	0 0 0 0 2	
1.500E-05	2.674E-03	ns	W005	0 0 1 2 1	

3212. C₁₄H₁₀

Anthracene
Paranaphthalene
Anthracin
Green oil
Anthraxcene

RN: 120-12-7 **MP (°C):** 218
MW: 178.24 **BP (°C):** 342

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.125E-08	1.270E-05	5.20	M063	2 1 2 2 2	
7.100E-08	1.265E-05	5.20	M082	1 1 1 2 1	
7.100E-08	1.265E-05	5.20	M151	2 1 2 2 1	
7.133E-08	1.271E-05	5.24	M183	1 2 1 1 2	
9.818E-08	1.750E-05	10.00	M063	2 1 2 2 2	
9.800E-08	1.747E-05	10.00	M082	1 1 1 2 1	
9.800E-08	1.747E-05	10.00	M151	2 1 2 2 1	
9.828E-08	1.752E-05	10.04	M183	1 2 1 1 2	
9.094E-08	1.621E-05	9.74	M183	1 2 1 1 2	
1.246E-07	2.220E-05	14.10	M063	2 1 2 2 2	
1.250E-07	2.228E-05	14.10	M082	1 1 1 2 2	
1.250E-07	2.228E-05	14.10	M151	2 1 2 2 2	
1.247E-07	2.223E-05	14.14	M183	1 2 1 1 2	
1.212E-07	2.160E-05	15	B385	0 0 0 0 0	
1.409E-07	2.512E-05	16.64	M183	1 2 1 1 2	
1.633E-07	2.910E-05	18.30	M063	2 1 2 2 2	
1.630E-07	2.905E-05	18.30	M082	1 1 1 2 2	
1.630E-07	2.905E-05	18.30	M151	2 1 2 2 2	
1.634E-07	2.912E-05	18.34	M183	1 2 1 1 2	
2.400E-07	4.278E-05	20	E009	1 0 0 0 1	
2.240E-07	3.992E-05	20	E025	1 0 2 2 2	
1.851E-07	3.300E-05	20	H300	1 1 2 2 1	

(continued)

3212. C₁₄H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.087E-07	3.720E-05	22.40	M063	2 1 2 2 2	
2.090E-07	3.725E-05	22.40	M082	1 1 1 2 2	
2.090E-07	3.725E-05	22.40	M151	2 1 2 2 2	
2.089E-07	3.723E-05	22.44	M183	1 2 1 1 2	
2.974E-07	5.300E-05	22.5	G301	0 0 0 0 0	
3.927E-07	7.000E-05	23	P332	0 0 0 0 0	
3.927E-07	7.000E-05	23	P339	0 0 0 0 0	
2.123E-07	3.784E-05	23.24	M183	1 2 1 1 2	
2.435E-07	4.340E-05	24.60	M063	2 1 2 2 2	
2.440E-07	4.349E-05	24.60	M082	1 1 1 2 2	
2.440E-07	4.349E-05	24.60	M151	2 1 2 2 2	
2.437E-07	4.344E-05	24.64	M183	1 2 1 1 2	
2.500E-07	4.456E-05	25	A325	2 1 2 2 1	
2.188E-07	3.900E-05	25	B319	2 0 1 2 1	average of 2
2.174E-07	3.875E-05	25	B385	0 0 0 0 0	
5.218E-07	9.300E-05	25	D406	1 2 2 2 2	
4.470E-07	7.967E-05	25	K001	2 2 2 2 2	
3.800E-07	6.773E-05	25	K123	1 0 2 2 1	
4.152E-07	7.400E-05	25	L301	1 1 2 2 2	
3.927E-07	7.000E-05	25	L332	1 1 1 1 2	
4.096E-07	7.300E-05	25	M064	1 1 2 2 1	
4.100E-06	7.308E-04	25	M342	1 0 1 1 2	
1.683E-07	3.000E-05	25	S227	1 2 1 1 1	
4.211E-07	7.506E-05	25	T066	1 0 0 0 2	
2.500E-07	4.456E-05	25	W300	2 2 2 2 2	
2.502E-07	4.460E-05	25.00	M151	2 1 1 2 2	
4.208E-07	7.500E-05	27	D003	1 0 0 1 1	
3.125E-07	5.570E-05	28.70	M063	2 1 2 2 2	
3.130E-07	5.579E-05	28.70	M082	1 1 1 2 2	
3.130E-07	5.579E-05	28.70	M151	2 1 2 2 2	
3.128E-07	5.575E-05	28.74	M183	1 2 1 1 2	
3.198E-07	5.700E-05	29	M071	2 2 2 2 2	
3.198E-07	5.700E-05	29.00	M151	2 1 1 2 2	
3.212E-07	5.724E-05	29.34	M183	1 2 1 1 2	
3.512E-07	6.260E-05	35	B385	0 0 0 0 0	
6.845E-07	1.220E-04	35.40	W003	2 2 2 2 2	average of 3
8.416E-07	1.500E-04	39.30	W003	2 2 2 2 2	average of 3
1.167E-06	2.080E-04	44.70	W003	2 2 2 2 2	average of 3
1.565E-06	2.790E-04	47.50	W003	2 2 2 2 2	
1.683E-06	3.000E-04	50.10	W003	2 2 2 2 2	average of 3
2.211E-06	3.940E-04	54.70	W003	2 2 2 2 2	average of 3
2.794E-06	4.980E-04	59.20	W003	2 2 2 2 2	average of 3
3.703E-06	6.600E-04	64.50	W003	2 2 2 2 1	average of 3
3.703E-06	6.600E-04	65.10	W003	2 2 2 2 1	average of 3
5.162E-06	9.200E-04	69.80	W003	2 2 2 2 1	
5.274E-06	9.400E-04	70.70	W003	2 2 2 2 1	average of 3
5.106E-06	9.100E-04	71.90	W003	2 2 2 2 2	
6.677E-06	1.190E-03	74.70	W003	2 2 2 2 2	average of 3
2.356E-07	4.200E-05	ns	H123	0 0 0 0 0	

(continued)

3212. C₁₄H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-07	3.208E-05	ns	H306	1 0 1 2 1	
4.096E-07	7.300E-05	ns	K304	0 0 0 0 1	
4.096E-07	7.300E-05	ns	M344	0 0 0 0 2	
5.000E-07	8.912E-05	ns	W005	0 0 1 2 0	

3213. C₁₄H₁₀Cl₂O₃

Fenclofenac

Benzeneacetic acid, 2-(2,4-dichlorophenoxy)-
RX 67408RN: 34645-84-6 MP (°C): 136
MW: 297.14 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.840E-05	8.439E-03	25	C314	0 0 0 0 0	
2.827E-05	8.400E-03	25	C314	0 0 0 0 0	

3214. C₁₄H₁₀Cl₄

DDD

1,1-Dichloro-2,2-bis(*p*-chlorophenyl)ethane*p,p'*-TDE

Dichlorodiphenyldichloroethane

RN: 72-54-8 MP (°C): 109.5
MW: 320.05 BP (°C): 193

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.562E-07	5.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
2.812E-07	9.000E-05	25	B083	2 2 1 2 1	particle size 5 µm
6.249E-08	2.000E-05	25	W025	1 0 2 2 1	
4.687E-07	1.500E-04	35	B083	2 2 1 2 2	particle size 5 µm
7.499E-07	2.400E-04	45	B083	2 2 1 2 2	particle size 5 µm
9.374E-09	3.000E-06	ns	M110	0 0 0 0 0	EFG

3215. C₁₄H₁₀Cl₄1-(2-Chlorophenyl)-1-(4-chlorophenyl)-2,2-dichloroethane
o,p'-DDDRN: 53-19-0 MP (°C): 76
MW: 320.05 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.875E-07	6.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
3.125E-07	1.000E-04	25	B083	2 2 1 2 2	particle size 5 µm
8.749E-07	2.800E-04	35	B083	2 2 1 2 2	particle size 5 µm
9.842E-07	3.150E-04	45	B083	2 2 1 2 2	particle size 5 µm

3216. C₁₄H₁₀F₃NO₂

Flufenamic acid

N-(α,α,α -Trifluoro-*m*-tolyl)anthranilic acid

N-(3-Trifluoromethylphenyl)anthranilic acid

RN: 530-78-9 **MP (°C):** 132–135**MW:** 281.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.890E-06	1.094E-03	25	G085	2 0 0 0 0	EFG
4.000E-05	1.125E-02	25	I007	1 2 2 2 0	EFG
1.031E-04	2.900E-02	30	D015	2 0 1 1 0	EFG
6.670E-06	1.876E-03	35	G085	2 0 0 0 0	EFG
6.200E-04	1.744E-01	35	H091	1 2 2 2 1	<i>sic</i>
2.133E-04	6.000E-02	37	D015	2 0 1 1 0	EFG
3.556E-05	1.000E-02	rt	H302	0 0 2 1 2	intrinsic

3217. C₁₄H₁₀N₂O₂

C.I. Disperse violet 1

1,4-Diamino-9,10-anthraquinone

Acetate red violet R

Acetoquinone light heliotrope NL

Supracet brilliant violet 3R

Violet 14447

RN: 128-95-0 **MP (°C):** 275**MW:** 238.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-07	2.287E-04	25	B333	0 0 0 0 0	

3218. C₁₄H₁₀N₂O₆

Dipentum

Olsalazine

RN: 15722-48-2 **MP (°C):****MW:** 302.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	1.149E-05	25	D311	0 0 0 0 0	0.1M NaCl

3219. C₁₄H₁₀O

2-Anthranol

2-Anthrol

RN: 613-14-9 **MP (°C):****MW:** 194.24 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.720E-04	9.167E-02	25	L085	1 2 0 1 2	

3220. C₁₄H₁₀O

1-Anthranol

1-Anthrol

Anthranol

RN: 529-86-2 MP (°C): 152

MW: 194.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	3.593E-02	25	L085	1 2 0 1 2	

3221. C₁₄H₁₀O₃

Diphenyleneglycollic acid

RN: MP (°C):

MW: 226.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.082E-02	2.448E+00	25	K040	1 0 2 1 2	

3222. C₁₄H₁₀O₄

Diphenic acid

1,1'-Biphenyl-2,2'-dicarboxylic acid

2,2'-Biphenyldicarboxylic acid

RN: 482-05-3 MP (°C): 228

MW: 242.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-03	1.260E+00	25	K040	1 0 2 1 2	

3223. C₁₄H₁₀O₄

Benzoyl peroxide

Benzoyl-peroxid

RN: 94-36-0 MP (°C): 105

MW: 242.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.399E-07	1.550E-04	rt	C342	0 0 0 0 0	

3224. C₁₄H₁₀O₅

Gentisin

9H-Xanthen-9-one, 1,7-dihydroxy-3-methoxy-

Gentianic acid

Gentianin

RN: 437-50-3**MP (°C):** 266.5**MW:** 258.23**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.162E-03	3.000E-01	16	F300	1 0 0 0 2	

3225. C₁₄H₁₀O₉

Digallic acid

m-Digallic acid*m*-Digallussaeure**RN:** 536-08-3**MP (°C):****MW:** 322.23**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.552E-03	5.000E-01	25	F300	1 0 0 0 0	
5.896E-02	1.900E+01	100	F300	1 0 0 0 1	

3226. C₁₄H₁₁CINO₂

7-Chloro-5,11-dihydrodibenz[b,e][1,4]oxazepine-5-carboxamide

RN:**MP (°C):****MW:** 260.70**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.534E-04	4.000E-02	37	G020	1 0 0 0 1	

3227. C₁₄H₁₁CIN₂O₄

2'-Methyl-3'chloro-2-hydroxy-5-nitrobenzanolide

Benzamide, *N*-(3-chloro-2-methyphenyl)-2-hydroxy-5-nitro-**RN:** 213460-66-3**MP (°C):****MW:** 306.71**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.102E-05	3.379E-03	25	D400	2 0 0 1 2	

3228. C₁₄H₁₁CIN₂O₄

2'-Methyl-5'-chloro-2-hydroxy-5-nitrobenzalide
 Benzamide, *N*-(5-chloro-2-methylphenyl)-2-hydroxy-5-nitro-
RN: 213460-65-2 **MP (°C):**
MW: 306.71 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.534E-06	2.311E-03	25	D400	2 0 0 1 2	

3229. C₁₄H₁₁CIN₂O₄

2'-Methyl-3'-chloro-2-hydroxy-3-nitrobenzalide
 Benzamide, *N*-(3-chloro-2methylphenyl)-2-hydroxy-3-nitro-
RN: 73544-88-4 **MP (°C):**
MW: 306.71 **BP (°C):** 324.7–408.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-05	4.685E-03	25	D400	2 0 0 1 2	

3230. C₁₄H₁₁CIN₂O₄

2'-Methyl-3'-chloro-2-hydroxy-3nitrobenzalide
 Benzamide, *N*-(5-chloro-2methylphenyl)-2-hydroxy-3-nitro-
RN: 213460-62-9 **MP (°C):**
MW: 306.71 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.528E-05	4.685E-03	25	D400	2 0 0 1 2	

3231. C₁₄H₁₁CIN₂O₄S

Chlorthalidone
 2-Chloro-5-(2,3-dihydro-1-hydroxy-3-oxo-1H-isoindol-1-yl)benzenesulfonamide
 Hygroton
 Thalitone
 Chlortalidone
RN: 77-36-1 **MP (°C):**
MW: 338.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.542E-04	1.200E-01	25	P312	0 0 0 0 0	
4.510E-04	1.528E-01	ns	I304	0 0 0 0 0	

3232. C₁₄H₁₁Cl₂NO₂

Diclofenac

2-[(2,6-Dichlorophenyl)amino]benzeneacetic acid

RN: 15307-86-5 MP (°C): 157

MW: 296.16 BP (°C): 412

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.317E-06	1.278E-03	30	P438	0 0 0 0 0	pH 2.0
1.182E-05	3.500E-03	32	C411	2 1 1 2 1	
4.478E-06	1.326E-03	33	P438	0 0 0 0 0	pH 2.0
5.117E-06	1.515E-03	37	P438	0 0 0 0 0	pH 2.0
5.389E-06	1.596E-03	39.5	P438	0 0 0 0 0	pH 2.0
5.822E-06	1.724E-03	42	P438	0 0 0 0 0	pH 2.0

3233. C₁₄H₁₁Cl₃O₂2,2-bis(*p*-Hydroxyphenyl)-1,1,1-trichloroethylene

Hydroxychlor

p,p'-Hydroxy-DDT

RN: 2971-36-0 MP (°C): 194

MW: 317.60 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.393E-04	7.600E-02	ns	K117	0 1 2 1 1	

3234. C₁₄H₁₁FN₂O₅

1-Acetoxyethyl-3-benzoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

1-Acetoxyethyl-3-benzoyl-5-fluorouracil

RN: 97096-67-8 MP (°C): 127–128

MW: 306.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.571E-04	1.400E-01	22	B321	0 0 0 0 0	pH 4.0

3235. C₁₄H₁₁N

2-Aminoanthracene

2-Anthrylamine

 β -Aminoanthracene

2-Anthracenamine

2-Anthramine

Anthracene amine

RN: 613-13-8 MP (°C): 238

MW: 193.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.727E-06	1.300E-03	24	H106	1 0 2 2 2	
6.727E-09	1.300E-06	ns	M349	0 2 1 1 2	

3236. C₁₄H₁₁N

Acetonitrile, diphenyl-
Diphenatrile

RN: 86-29-3 **MP (°C):** 74
MW: 193.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.138E-03	2.200E-01	ns	B185	0 0 0 0 0	

3237. C₁₄H₁₁NO₂

N-Benzoylbenzamide
Dibenzamid

RN: 614-28-8 **MP (°C):** 152
MW: 225.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.327E-03	1.200E+00	15	F300	1 0 0 0 1	

3238. C₁₄H₁₁N₃O₂

Salicyloylhydrazone of picolinealdehyde

RN: **MP (°C):**
MW: 253.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.897E-04	2.000E-01	ns	G089	0 1 2 0 1	

3239. C₁₄H₁₂

1-Methylfluorene
1-Methyl-9H-fluorene

RN: 1730-37-6 **MP (°C):** 87
MW: 180.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.047E-06	1.090E-03	25	B319	2 0 1 2 2	
6.060E-06	1.092E-03	25	M342	1 0 1 1 2	

3240. C₁₄H₁₂

1,1-Diphenylethene
1,1-Diphenylethylene

RN: 530-48-3 **MP (°C):** 8.2
MW: 180.25 **BP (°C):** 277

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.662E-05	6.600E-03	25	A002	1 0 1 1 1	

3241. C₁₄H₁₂

9,10-Dihydroanthracene

RN: 613-31-0

MP (°C): 104–107

MW: 180.25

BP (°C): 312

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.578E-06	4.646E-04	4.96	R423	0 0 0 0 0	
2.622E-06	4.727E-04	5.85	R423	0 0 0 0 0	
2.917E-06	5.257E-04	7.95	R423	0 0 0 0 0	
3.317E-06	5.978E-04	10.95	R423	0 0 0 0 0	
3.556E-06	6.409E-04	12.05	R423	0 0 0 0 0	
4.261E-06	7.681E-04	14.95	R423	0 0 0 0 0	
4.961E-06	8.942E-04	18.00	R423	0 0 0 0 0	
5.811E-06	1.047E-03	20.96	R423	0 0 0 0 0	
7.389E-06	1.332E-03	24.59	R423	0 0 0 0 0	
8.011E-06	1.444E-03	26.59	R423	0 0 0 0 0	
9.400E-06	1.694E-03	29.05	R423	0 0 0 0 0	
1.114E-05	2.009E-03	32.66	R423	0 0 0 0 0	
1.288E-05	2.321E-03	36.28	R423	0 0 0 0 0	
1.498E-05	2.701E-03	40.01	R423	0 0 0 0 0	

3242. C₁₄H₁₂*trans*-Stilbene*trans*-Diphenylethylene

1,2-Diphenylethene

trans-1,2-Diphenylethylene*trans*-α, β-Diphenylethylene

Toluylene

RN: 103-30-0

MP (°C): 124

MW: 180.25

BP (°C): 306

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.609E-06	2.900E-04	25	A002	1 0 1 1 1	

3243. C₁₄H₁₂F₃NO₄S₂

Perfluidone

Methyl-4-(phenylsulfonyl)trifluoromethanesulfonanilide

1,1,1-Trifluoro-N-(2-methyl-4-(phenylsulfonyl)phenyl)methanesulfonamide

Destun

MBR 8251

Trifluoro-N-(2-methyl-4-(phenylsulfonyl)phenyl)methanesulfonamide

RN: 37924-13-3 MP (°C): 143

MW: 379.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.582E-04	6.000E-02	22	G306	1 0 0 1	
1.582E-04	6.000E-02	22	M161	1 0 0 1	

3244. C₁₄H₁₂N₂O₄

4'-Methyl-2-hydroxy-5-nitrobenzanilide

Benzamide, 2-hydroxy-*N*-(4-methylphenyl)-5-nitro-

RN: 68507-96-0 MP (°C):

MW: 272.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-05	3.846E-03	25	D400	2 0 0 1 2	

3245. C₁₄H₁₂N₂O₄

4'-Methyl-2-hydroxy-3-nitrobenzanilide

Benzamide, 2-hydroxy-*N*-(4-methylphenyl)-3-nitro-

RN: 68507-90-4 MP (°C):

MW: 272.26 BP (°C): 305.7–389.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.069E-05	8.356E-03	25	D400	2 0 0 1 2	

3246. C₁₄H₁₂N₂O₄

2'-Methyl-2-hydroxy-3-nitrobenzanilide

Benzamide, 2-hydroxy-*N*-(2-methylphenyl)-3-nitro-

RN: 68507-89-1 MP (°C):

MW: 272.26 BP (°C): 302–384.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.818E-05	7.673E-03	25	D400	2 0 0 1 2	

3247. C₁₄H₁₂N₂O₅

4'-Methoxy-2-hydroxy-5-nitrobenzanilide

p-Salicylaniside, 5-nitro-Benzamide, 2-hydroxy-*N*-(4-methoxyphenyl)-5-nitro-

RN: 68507-94-8 MP (°C):

MW: 288.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.928E-05	5.556E-03	25	D400	2 0 0 1 2	

3248. C₁₄H₁₂N₂O₅

4'-Methoxy-2-hydroxy-3-nitrobenzanilide

Benzamide, 2-hydroxy-*N*-(4-methoxyphenyl)-3-nitro-

RN: 68507-88-0 MP (°C):

MW: 288.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.532E-05	1.018E-02	25	D400	2 0 0 1 2	

3249. C₁₄H₁₂N₂S

2-(4-Aminophenyl)-6-methyl-benzothiazole

Dehydrothio-*N*-toluidinDehydrothio-*N*-toluidine

RN: 92-36-4 MP (°C): 194.8

MW: 240.33 BP (°C): 434

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.080E-04	5.000E-02	100	F300	1 0 0 0 0	

3250. C₁₄H₁₂N₄O₂

C.I. Disperse blue 1

9,10-Anthracenedione, 1,4,5,8-tetraamino-

RN: 2475-45-8 MP (°C): 332

MW: 268.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-07	2.683E-05	25	B333	0 0 0 0 0	

3251. C₁₄H₁₂O₂

4-Biphenylacetic acid

Felbinac

RN: 5728-52-9 MP (°C):

MW: 212.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	3.927E-02	25	P344	0 0 0 0 0	EFG

3252. C₁₄H₁₂O₂

Benzoin

2-Hydroxy-1,2-diphenylethanone

Benzoylphenylcarbinol

2-Hydroxy-2-phenylacetophenone

Hydroxy-2-phenyl acetophenone

RN: 579-44-2 MP (°C): 137

MW: 212.25 BP (°C): 344

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-03	3.000E-01	25	F300	1 0 0 0 0	
1.413E-03	2.999E-01	rt	D021	0 0 1 1 0	

3253. C₁₄H₁₂O₂

Benzyl benzoate

Ascabin

Scabagen

Benzoic acid phenylmethyl ester

Benylate

Phenylmethyl benzoate

RN: 120-51-4 **MP (°C):** 19
MW: 212.25 **BP (°C):** 323

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.225E-04	2.600E-02	15	H069	1 0 1 1 1	
6.960E-03	1.477E+00	30	M444	0 0 0 0 0	
7.020E-03	1.490E+00	40	M444	0 0 0 0 0	
7.150E-03	1.518E+00	50	M444	0 0 0 0 0	
7.230E-03	1.535E+00	60	M444	0 0 0 0 0	

3254. C₁₄H₁₂O₂

Diphenylacetic acid

Diphenyl-essigsaeure

RN: 117-34-0 **MP (°C):** 148
MW: 212.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-04	1.274E-01	25	K040	1 0 2 1 2	

3255. C₁₄H₁₂O₃

Benzilic acid

2,2-Diphenyl-2-hydroxyacetic acid

Diphenylglycolic acid

Benzeneacetic acid, α -hydroxy- α -phenyl-

2-Hydroxy-2,2-diphenylethanoic acid

RN: 76-93-7 **MP (°C):** 150
MW: 228.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.690E-03	1.755E+00	25	K040	1 0 2 1 2	
6.190E-03	1.413E+00	25	L050	2 0 1 2 2	

3256. C₁₄H₁₂O₃

Benzylparaben

Benzyl 4-hydroxybenzoate

Phenylmethyl ester

RN: 94-18-8**MP (°C):****MW:** 228.25**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.031E-04	9.200E-02	25	P013	0 0 0 0 0	

3257. C₁₄H₁₂O₅

Khellin

Amicardine

RN: 82-02-0**MP (°C):** 154.5**MW:** 260.25**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.500E-01	2.472E+02	25	E312	0 0 0 0 0	EFG, <i>sic</i>
1.153E-04	3.000E-02	25	J028	1 2 0 2 0	
7.000E-04	1.822E-01	30	E012	1 2 1 1 0	
1.300E-03	3.383E-01	42	E012	1 2 1 1 0	

3258. C₁₄H₁₃ClN₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 2-chloro-11-ethyl-5,11-dihydro-5-methyl-

RN: 133627-12-0 **MP (°C):****MW:** 288.74**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.691E-05	2.221E-02	ns	M381	0 1 1 1 2	pH 7.0

3259. C₁₄H₁₃NO₆

Benzoic acid, 2-(acetoxy)-, (2,5-dioxo-1-pyrrolidinyl)methyl ester

Salicylic acid acetate, ester with *N*-(hydroxymethyl)succinimide**RN:** 32620-72-7 **MP (°C):** 117.5**MW:** 291.26**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.717E-03	5.000E-01	21	N335	0 0 0 0 0	

3260. C₁₄H₁₃N₂

4,7-Dimethyl-1,10-phenanthroline

4,7-Dimethyl-*o*-phenanthroline

RN: 3248-05-3 **MP (°C):** 193
MW: 209.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E-04	2.239E-02	25.04	B094	1 2 1 2 2	

3261. C₁₄H₁₃N₃O₂Pyrido[2,3-*b*][1,5]benzoxazepin-5(6H)-one, 3-amino-6,9-dimethyl-

RN: 134894-45-4 **MP (°C):**
MW: 255.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.057E-04	2.312E-01	ns	M381	0 1 1 1 2	pH 7.0

3262. C₁₄H₁₃N₃O₄S₂

Meloxicam

RN: 71125-38-7 **MP (°C):**
MW: 351.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	2.284E-02	25	C434	0 0 0 0 0	pH 6.0
3.415E-05	1.200E-02	25	S415	0 0 0 0 0	
9.500E-05	3.338E-02	30	C434	0 0 0 0 0	pH 6.0
1.550E-05	5.447E-03	37	C434	0 0 0 0 0	pH 6.0
3.699E-06	1.300E-03	37	Y421	0 0 0 0 0	
2.800E-05	9.839E-03	45	C434	0 0 0 0 0	pH 6.0

3263. C₁₄H₁₄

4,4'-Dimethylbiphenyl

4,4'-Dimethyl-1,1'-biphenyl

p,p'-Bitoluene

RN: 613-33-2 **MP (°C):** 125.0
MW: 182.27 **BP (°C):** 295.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.770E-07	6.871E-05	4.0	D330	2 2 1 2 2	
9.590E-07	1.748E-04	25.0	D330	2 2 1 2 2	
2.420E-06	4.411E-04	40.0	D330	2 2 1 2 2	

3264. C₁₄H₁₄

Bibenzyl

1,2-Diphenylethane

Benzene, 1,1'-(1,2-ethanediyl)*bis*-

RN: 103-29-7 MP (°C): 52.0

MW: 182.27 BP (°C): 284

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.359E-05	4.300E-03	25	A002	1 0 1 1 1	

3265. C₁₄H₁₄NO₄PS

EPN

Ethyl *O*-(*p*-nitrophenyl) phenylphosphonothionate*O*-Ethyl *O*-*p*-nitrophenyl benzenephosphonothioateEthyl *O*-(*p*-nitrophenyl) benzenethiophosphonate

RN: 2104-64-5 MP (°C): 36

MW: 323.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.629E-06	3.113E-03	22	K137	1 1 2 1 0	

3266. C₁₄H₁₄N₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-5-methyl

RN: 132312-85-7 MP (°C):

MW: 254.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.399E-03	6.100E-01	ns	M381	0 1 1 1 2	pH 7.0

3267. C₁₄H₁₄N₄O₂

Dis. A. 7

RN: 2491-74-9 MP (°C): 236

MW: 270.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-09	5.406E-07	25	B333	0 0 0 0 0	

3268. C₁₄H₁₄N₄O₂

Dye II

4-[[4-Dimethylamino)phenyl]azo]nitrobenzene

RN: MP (°C):

MW: 270.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.800E-07	2.108E-04	84.10	B198	1 2 1 1 1	
2.040E-06	5.514E-04	97.40	B198	1 2 1 1 2	

3269. C₁₄H₁₄N₄O₄ β,γ -Dihydroxypropyltheophylline**RN:** 180262-60-6 **MP (°C):****MW:** 302.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.007E-01	9.091E+01	ns	J025	0 0 0 0 1	

3270. C₁₄H₁₄N₄S

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepine-6-thione, 11-ethyl-5,11-dihydro-5-methyl

RN: 134698-27-4 **MP (°C):****MW:** 270.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.323E-05	6.280E-03	ns	M381	0 1 1 1 2	pH 7.0

3271. C₁₄H₁₄O6-Benzyl-*m*-cresol

Phenol, 5-methyl-2-(phenylmethyl)-

RN: 30091-04-4 **MP (°C):****MW:** 198.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.441E-04	2.857E-02	25	L021	1 0 0 0 0	

3272. C₁₄H₁₄O

DL-1,2-Diphenylethanol

DL-1,2-Diphenyl-aethanol

RN: 614-29-9 **MP (°C):** 67**MW:** 198.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.026E-03	6.000E-01	100	F300	1 0 0 0 0	

3273. C₁₄H₁₄O₂

DL-Hydrobenzoin

Hydrobenzoin

RN: 27134-24-3 **MP (°C):** 139**MW:** 214.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.167E-02	2.500E+00	15	F300	1 0 0 0 1	
8.867E-03	1.900E+00	15	F300	1 0 0 0 1	
6.021E-02	1.290E+01	100	F300	1 0 0 0 2	

3274. C₁₄H₁₄O₃

Pindone

2-Pivaloylindandione-1,3

RN: 83-26-1

MP (°C): 109

MW: 230.27

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.817E-05	1.800E-02	25	M061	1 0 0 0 1	
7.817E-05	1.800E-02	25	M161	1 0 0 0 1	

3275. C₁₄H₁₄O₃

Naproxen

6-Methoxy- α -methyl-2-naphthaleneacetic acid(S)-6-Methoxy- α -methyl-2-naphthaleneacetic acid

Laraflex

RN: 22204-53-1 MP (°C): 155.3

MW: 230.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.310E-05	9.924E-03	5	F306	1 0 1 2 2	intrinsic
6.948E-05	1.600E-02	21	B331	1 2 2 1 2	pH 7.4
6.080E-05	1.400E-02	25	A408	2 0 1 2 0	int
6.905E-05	1.590E-02	25	A427	0 0 0 0 0	
6.905E-05	1.590E-02	25	C059	1 2 1 1 2	
6.900E-05	1.589E-02	25	F306	1 0 1 2 2	intrinsic
1.146E-04	2.639E-02	37	F306	1 0 1 2 2	intrinsic
2.171E-05	5.000E-03	37	Y421	0 0 0 0 0	
5.211E-04	1.200E-01	amb	L434	0 0 0 0 0	
5.646E-05	1.300E-02	rt	H302	0 0 2 1 2	intrinsic

3276. C₁₄H₁₄O₃S*o*-Cresyl-*p*-toluene sulfonate

2-Methylphenyl tosylate

o-Tolyl tosylate

2-Tolyl tosylate

RN: 599-75-7 MP (°C):

MW: 262.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.144E-04	3.000E-02	ns	F014	0 0 0 0 0	

3277. C₁₄H₁₄O₄Diallyl *m*-phthalate

RN:

MP (°C):

MW: 246.27

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.990E-04	4.900E-02	25	S417	0 0 0 0 0	

3278. C₁₄H₁₄O₄

Diallyl phthalate

Di-2-propenyl phthalate

RN: 131-17-9

MP (°C): -70

MW: 246.27

BP (°C): 165

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.06E-04	<10.00E-02	20	F070	1 0 0 0 1	
7.390E-04	1.820E-01	20	L300	2 1 0 2 2	
7.413E-04	1.826E-01	ns	S460	0 0 0 0 0	

3279. C₁₄H₁₅N*p*-Aminostilbene

4-Aminostilbene

RN: 834-24-2

MP (°C):

MW: 197.28

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.534E-05	5.000E-03	rt	N015	0 0 2 2 0	

3280. C₁₄H₁₅NO₅

L-Proline, 1-[(benzoyloxy)acetyl]-

RN: 115178-75-1 MP (°C): 72.5

MW: 277.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.561E-02	7.100E+00	22	N317	1 1 2 1 2	

3281. C₁₄H₁₅N₃*o*-Aminoazotoluene

2-Amino-5-azotoluene

RN: 97-56-3 MP (°C): 101

MW: 225.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.107E-05	7.000E-03	37	H120	1 1 1 1 1	normal saline

3282. C₁₄H₁₅N₃*p*-Dimethylaminoazobenzene

4-Dimethylaminoazobenzol

Dimethylaminoazobenzene

Methylgelb

C. I. Solvent yellow 2

RN: 60-11-7 **MP (°C):** 116
MW: 225.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.877E-04	2.000E-01	20	F300	1 0 0 0 0	
6.214E-06	1.400E-03	20	J027	1 0 0 0 1	
1.700E-06	3.830E-04	25	B333	0 0 0 0 0	<i>sic</i>
1.775E-06	4.000E-04	30	R430	0 0 0 0 0	
7.101E-04	1.600E-01	rt	D021	0 0 1 1 1	<i>sic</i>

3283. C₁₄H₁₅N₃O₃S

Gly-dapsone

Acetamide, 2-amino-N-[4-[(4-aminophenyl)sulfonyl]phenyl]

RN: 160349-02-0 **MP (°C):**
MW: 305.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.849E-03	8.700E-01	25	P351	0 0 0 0 0	
>4.91E-02	>1.50E+01	25	P351	0 0 0 0 0	pH 7.4

3284. C₁₄H₁₅N₅O₅9-(2-*O*-Butyryl-β-D-arabinofuranosyl)adenine9H-Purin-6-amine, 9-[3,5-*bis*-*O*-[(1,1-dimethylethyl)dimethylsilyl]-2-*O*-(1-oxobutyl)-β-D-arabinofuranosyl]-

RN: 87970-05-6 **MP (°C):**
MW: 333.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.023E-04	3.410E-02	37	B306	1 2 0 1 2	pH 7.3

3285. C₁₄H₁₅N₅O₆S

Metasulfron-methyl

Metsulfuron methyl ester

Allie

Escort

DPX-T6376

Ally

RN: 74223-64-6 **MP (°C):** 158

MW: 381.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.079E-05	2.700E-02	ns	R427	0 0 0 0 0	

3286. C₁₄H₁₅O₂PS₂

Edifenphos

RN: 17109-49-8 **MP (°C):**
MW: 310.38 **BP (°C):** 154

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.803E-04	5.596E-02	ns	S460	0 0 0 0 0	

3287. C₁₄H₁₆CIN₃O₂

Triadimefon

1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone

Triamefon

Bayleton

RN: 43121-43-3 **MP (°C):** 82.3
MW: 293.76 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.851E-04	2.600E-01	20	M161	1 0 0 0 2	

3288. C₁₄H₁₆ClO₅PS

Coumaphos

O,O-Diethyl O-(3-chloro-4-methylcoumarinyl-7) thiophosphate

RN: 56-72-4 **MP (°C):** 91
MW: 362.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.135E-06	1.500E-03	20	M061	1 0 0 0 1	
4.169E-06	1.512E-03	ns	R427	0 0 0 0 0	

3289. C₁₄H₁₆Cl₂O₃

2,4-Dichlorophenoxyacetic acid cyclohexyl ester

Cyclohexyl 2,4-dichlorophenoxyacetate

RN: 65267-97-2 **MP (°C):**
MW: 303.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.811E-05	5.492E-03	ns	M120	0 0 1 1 2	

3290. C₁₄H₁₆FN₃O₃

2,5-Diaziridinyl-3-floro-6-morpholino-1,4-benzoquinone

2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1-aziridinyl)-3-fluoro-6-(4-morpholinyl)-

RN: 59886-45-2 **MP (°C):** 157
MW: 293.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.819E-03	2.000E+00	rt	C317	0 0 0 0 0	

3291. C₁₄H₁₆F₃N₃O₄

Profluralin

N-(Cyclopropylmethyl)-2,6-dinitro-*N*-propyl-4-(trifluoromethyl)benzenamine

Pregard

Tolban

ER-5461

RN: 26399-36-0 **MP (°C):** 32
MW: 347.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.879E-07	1.000E-04	20	E048	1 2 1 1 0	
2.879E-07	1.000E-04	20	M161	1 0 0 0 0	
2.879E-07	1.000E-04	27	K315	1 0 0 0 1	

3292. C₁₄H₁₆N₂*o*-Tolidine

3,3'-Dimethylbenzidine

RN: 119-93-7 **MP (°C):** 130.0
MW: 212.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.123E-03	1.300E+00	25	B068	2 0 1 1 1	

3293. C₁₄H₁₆N₂O₂

3,3'-Dimethoxybenzidine

o-Dianisidine

Dianisidine

RN: 119-90-4 **MP (°C):** 137
MW: 244.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.456E-04	6.000E-02	25	B068	2 0 1 1 0	

3294. C₁₄H₁₆N₂O₄

2-Pyrrolidinecarboxamide, 1-[(benzoyloxy)acetyl]-

RN: 116482-82-7 **MP (°C):** 194.5
MW: 276.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.429E-03	1.500E+00	22	N317	1 1 2 1 2	

3295. C₁₄H₁₆N₂O₄

2-Pyrrolidinecarboxamide, 1-[(benzoyloxy)acetyl]-

RN: 106231-69-0 MP (°C):

MW: 276.29 BP (°C): 570.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.429E-03	1.500E+00	22	B427	1 0 0 1 1	

3296. C₁₄H₁₆N₂O₄S₂4-Thiazolidinecarboxylic acid, 2,2'-(1,4-phenylene)*bis*-4-Thiazolidinecarboxylic acid, 2,2'-*p*-phenylenebis-

RN: 83690-84-0 MP (°C):

MW: 340.42 BP (°C): 697.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-03	6.128E-01	21	B414	1 0 0 1 1	fast decomposition

3297. C₁₄H₁₆N₄

Disperse black 3

N,N-Dimethyl-4,4'-azodian

4-Amino-4'-(dimethylamino)azobenzene

C.I. 11025

RN: 539-17-3 MP (°C):

MW: 240.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	1.202E-04	25	B333	0 0 0 0 0	

3298. C₁₄H₁₆N₄O₂S

2-Sulfanilamido-5,6,7,8-tetrahydroquinazoline

2-Sulfanilamido-5,6,7,8,-tetrahydroquinazoline

RN: 71119-34-1 MP (°C): 255

MW: 304.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.234E-04	6.800E-02	29	C049	0 0 0 0 0	

3299. C₁₄H₁₆N₄O₃S*N*4-Acetyl sulfamethazine*N*4-Acetyl sulfamezathine*N*4-Acetyl sulphamethazine

Acetyl sulfamethazine

2-*p*-Acetamido benzenesulphonamido-4:6-dimethylpyri-**RN:** 100-90-3 **MP (°C):****MW:** 320.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.900E-03	9.291E-01	37	G026	1 0 1 1 0	EFG, pH 5.4
3.590E-03	1.150E+00	37	L091	1 0 0 0 2	pH 5.5
3.590E-03	1.150E+00	37	M057	1 0 0 0 2	pH 5.5
3.590E-03	1.150E+00	37	R075	1 2 0 0 2	
2.197E-03	7.040E-01	37	S192	1 0 1 1 2	pH 6.0
2.622E-03	8.400E-01	38	K006	1 0 0 0 1	

3300. C₁₄H₁₆N₄O₃S*N*4-Acetyl sulphasomidineAcetamide, *N*-[4-[(2,6-dimethyl-4-pyrimidinyl)amino]sulfonyl]phenyl]-**RN:** 3163-31-3 **MP (°C):****MW:** 320.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.373E-04	4.400E-02	ns	B133	0 2 0 0 1	pH 7.4

3301. C₁₄H₁₆N₄O₃S2-(*N*4-Acetyl sulfamylamino)-4-ethylpyrimidine**RN:** **MP (°C):****MW:** 320.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.435E-05	7.800E-03	37	R076	1 2 0 0 2	

3302. C₁₄H₁₆N₄O₄S*N*4-Acetyl sulphamethomidine**RN:** **MP (°C):****MW:** 336.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.730E-04	2.600E-01	ns	B133	0 2 0 0 2	pH 7.4

3303. C₁₄H₁₆N₄O₅S

N4-Acetyl sulphadimethoxine

N4-Acetyl-2,4-dimethoxy-6-sulfanilamido pyrimidine

N4-Acetyl sulfadimethoxy pyrimidine

Sulfadimethoxine N4-acetate

RN: 555-25-9 MP (°C):

MW: 352.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.392E-04	1.900E-01	ns	B133	0 2 0 0 2	pH 7.4

3304. C₁₄H₁₆O₆

Benzoic acid, 2-(acetoxy)-, (1-oxobutoxy)methyl ester

RN: 118247-07-7 MP (°C): oil

MW: 280.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.249E-03	3.500E-01	21	N335	0 0 0 0 0	

3305. C₁₄H₁₆O₆

Ethylphthalyl ethyl glycolate

Ethoxycarbonylmethyl ethyl phthalate

Ethylphthalyl ethylglycolate

RN: 84-72-0 MP (°C): 20

MW: 280.28 BP (°C): 320

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.85E-03	<7.99E-01	20	F070	1 0 0 0 1	

3306. C₁₄H₁₇ClNO₄PS₂

Dialifos

Dialifor

Diethyl S-(2-chloro-1-phthalimidoethyl) phosphorodithioate

Torak

Hercules 14503

RN: 10311-84-9 MP (°C): 67

MW: 393.85 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.570E-07	1.800E-04	ns	F071	0 1 2 1 1	
4.571E-07	1.800E-04	ns	R427	0 0 0 0 0	

3307. C₁₄H₁₇NO

1-Cinnamoylpiperidine

N,N-Pentamethylenecinnamamide

1-(1-Oxo-3-phenyl-2-propenyl)-piperidine

RN: 5422-81-1 **MP (°C):****MW:** 215.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.600E-04	2.067E-01	ns	H350	0 0 0 0 0	

3308. C₁₄H₁₇NO

N-Cyclopentylcinnamamide

2-Propenamide, *N*-cyclopentyl-3-phenyl-**RN:** 59831-97-9 **MP (°C):****MW:** 215.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.280E-04	4.909E-02	ns	H350	0 0 0 0 0	

3309. C₁₄H₁₇NO₂S*m*-Carboxylhexylphenylisothiocyanate

3-Carboxylhexylphenylisothiocyanate

RN: **MP (°C):****MW:** 263.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.844E-02	25	K032	2 2 0 1 1	

3310. C₁₄H₁₇NO₃

Piperidine, 1-[(benzoyloxy)acetyl]-

RN: 106231-67-8 **MP (°C):** 88**MW:** 247.30 **BP (°C):** 433.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.154E-03	7.800E-01	22	B427	1 0 0 1 1	
3.154E-03	7.800E-01	22	N317	1 1 2 1 2	

3311. C₁₄H₁₇NO₄

4-Piperidinol, 1-[(benzoyloxy)acetyl]-

RN: 115178-71-7 **MP (°C):** 121.5**MW:** 263.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.482E-02	1.180E+01	22	N317	1 1 2 1 2	

3312. C₁₄H₁₇NO₅Glycine, *N*-[(benzoyloxy)acetyl]-*N*-methyl-, ethyl ester

RN: 106231-63-4 **MP (°C):** 39.5
MW: 279.30 **BP (°C):** 426.4

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.148E-02	6.000E+00	22	B427	1 0 0 1 1	
2.148E-02	6.000E+00	22	N317	1 1 2 1 2	in 0.01M HCl

3313. C₁₄H₁₇N₅O₃

Pipemidic acid

Pipemidique acide

RN: 51940-44-4 **MP (°C):** 253
MW: 303.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-03	3.215E-01	25	D051	2 0 0 1 2	0.05N NaCl
1.160E-03	3.519E-01	37	D051	2 0 0 1 2	0.05N NaCl

3314. C₁₄H₁₈ClN₃S

Chlorothen

N,N-Dimethyl-*N'*-(2-pyridyl)-*N'*-(5-chloro-2-thenyl)ethylenediamine

Chloromethapyrilene

5-Chloro-*N*-(2-(dimethylamino)ethyl)-*N*-(2-pyridyl)-2-thenylamine

Chloropyrilen

RN: 148-65-2 **MP (°C):**
MW: 295.84 **BP (°C):** 155.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-03	2.012E+00	37.5	L034	2 2 0 1 2	pH 7.4

3315. C₁₄H₁₈Cl₂O₃2,4-Dichlorophenoxyacetic acid *n*-hexyl ester

Chloroxone

AgroTECT

Amoxone

BH 2,4-D

RN: 1917-95-9 **MP (°C):**
MW: 305.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.941E-05	5.924E-03	ns	M120	0 0 1 1 2	

3316. C₁₄H₁₈N₂O

Propyphenazone

Isopropylantipyrine

1,2-Dihydro-1,5-dimethyl-4-(isopropyl)-2-phenyl-pyrazol-3-one

4-Isopropyl-2,3-dimethyl-5-oxo-1-phenyl-3-pyrazoline

RN: 479-92-5 MP (°C): 103

MW: 230.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.383E+00	7.791E+02	4.62	M109	2 1 1 1 0	EFG
3.330E+00	7.670E+02	10.93	M109	2 1 1 1 0	EFG
3.257E+00	7.501E+02	15.02	M109	2 1 1 1 0	EFG
3.238E+00	7.458E+02	20.96	M109	2 1 1 1 0	EFG
3.229E+00	7.436E+02	25.35	M109	2 1 1 1 0	EFG
3.238E+00	7.458E+02	29.87	M109	2 1 1 1 0	EFG
3.257E+00	7.501E+02	38.37	M109	2 1 1 1 0	EFG
3.348E+00	7.711E+02	40.32	M109	2 1 1 1 0	EFG

3317. C₁₄H₁₈N₂O₃

Reposal

5-Bicyclo[3.2.1]oct-2-en-3-yl-5-ethyl-2,4,6(1H,3H,5H)-pyrimidinetri-one

5-Bicyclo[3.2.1]oct-2-en-3-yl-5-ethylbarbituric acid

RN: 3625-25-0 MP (°C): 213

MW: 262.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.680E-03	4.407E-01	25	V033	2 0 1 1 2	
1.700E-03	4.459E-01	25.00	T303	1 0 0 0 1	
2.300E-03	6.033E-01	35.00	T303	1 0 0 0 1	
2.500E-03	6.558E-01	45.00	T303	1 0 0 0 1	

3318. C₁₄H₁₈N₂O₃

Piperazine, 1-[(benzoyloxy)acetyl]-4-methyl-

RN: 106231-70-3 MP (°C):

MW: 262.31 BP (°C): 438.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>7.62E-01	>2.00E+02	22	B427	1 0 0 1 1	

3319. C₁₄H₁₈N₄O₂S

2-Sulfanilylmino-4-isobutylpyrimidine

RN: 106596-34-3 MP (°C):

MW: 306.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.264E-04	1.000E-01	37	R076	1 2 0 0 1	

3320. C₁₄H₁₈N₄O₃

Benomyl

(1-(Butylamino)carbonyl)-1H-benzimidazol-2-yl)carbamic acid methyl ester

RN: 17804-35-2 **MP (°C):****MW:** 290.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.309E-05	3.800E-03	20	A064	1 0 1 1 1	
1.309E-05	3.800E-03	20	M161	1 0 0 0 1	pH 7
~6.89E-06	~2.00E-03	ns	B309	0 0 0 0 0	

3321. C₁₄H₁₈N₄O₃

Trimethoprim

5-(3,4,5-Trimethoxybenzyl)-2,4-diaminopyrimidine

Monotrim

Syraprim

Proloprim

Trimpex

RN: 738-70-5 **MP (°C):** 201**MW:** 290.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.034E-05	1.752E-02	22.5	B440	0 0 0 0 0	
1.396E-03	4.053E-01	25	H434	0 0 0 0 0	
1.378E-03	4.000E-01	25	M167	1 0 0 0 0	
1.722E-03	5.000E-01	32	D308	0 0 0 0 0	pH 8.54
2.711E-03	7.870E-01	37	G086	1 0 0 0 1	
1.378E-03	4.000E-01	37	M321	1 0 0 0 2	intrinsic
>1.72E-03	>5.00E-01	ns	B404	0 2 1 1 0	
1.378E-03	4.000E-01	ns	K444	0 0 0 0 0	

3322. C₁₄H₁₈N₄O₆.0.5H₂O

2'-Propionyl-6-methoxypurine arabinoside (hemihydrate)

RN: 145913-38-8 **MP (°C):** 60–65**MW:** 347.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-01	3.821E+01	37	C348	0 0 0 0 0	pH 7.00

3323. C₁₄H₁₈N₄O₇.0.5H₂O

9-[5-O-(Methoxyacetate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)

RN: 121032-38-0 **MP (°C):** 137–139**MW:** 363.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.810E-02	2.838E+01	37	M378	1 2 1 1 2	pH 7.2

3324. C₁₄H₁₈N₄O₇.0.9H₂O

2'-Methoxyacetyl-6-methoxypurine arabinoside (0.9 hydrate)

RN: 145913-47-9 MP (°C):

MW: 370.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.090E-02	3.368E+01	37	C348	0 0 0 0 0	pH 7.00

3325. C₁₄H₁₈N₆O

(1S,4R)-4-[2-Amino-6-(cyclopropylamino)-9H-purin-9-yl]-2-cyclopentene-1-methanol sulfate (salt)

ABC sulfate[47]

ABC[48]

Abacavir

RN: 188062-50-2 MP (°C):

MW: 286.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.867E-09	1.680E-06	32	M458	0 0 0 0 0	

3326. C₁₄H₁₈N₆O₄

2,5-Diaziridinyl-3,6-bis(glycinamide)-1,4-benzoquinone

RN: 59886-49-6 MP (°C): 200

MW: 334.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.495E-03	5.000E-01	rt	C317	0 0 0 0 0	

3327. C₁₄H₁₈O₄

Diisopropyl phthalate

bis(1-Methyl-ethyl) phthalate

RN: 605-45-8 MP (°C):

MW: 250.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-03	3.329E-01	20	L300	2 1 0 2 2	

3328. C₁₄H₁₈O₄Di-*n*-propyl phthalate

Dipropyl phthalate

RN: 131-16-8

MP (°C):

MW: 250.30

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-04	1.081E-01	20	L300	2 1 0 2 2	

3329. C₁₄H₁₈O₄Diisopropyl *o*-phthalate

RN: 131-16-8

MP (°C):

MW: 250.30

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.672E-04	1.670E-01	25	S417	0 0 0 0 0	

3330. C₁₄H₁₈O₆

Methyl glycol phthalate

bis(2-Methoxyethyl) phthalate

RN: 117-82-8

MP (°C):

MW: 282.30

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.090E-02	8.723E+00	15	H069	1 0 1 1 1	

3331. C₁₄H₁₈O₆

Ethyl phthalyl ethyl glycolate

RN: 117-82-8

MP (°C):

MW: 282.30

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.770E-03	4.998E-01	15	H069	1 0 1 1 0	
1.770E-03	4.998E-01	ns	F014	0 0 0 0 1	

3332. C₁₄H₁₈O₆

Dimethoxyethyl phthalate

1,2-Benzenedicarboxylic acid, di(2-methoxyethyl) ester

RN: 34006-76-3

MP (°C):

MW: 282.30

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.986E-02	8.428E+00	20	F070	1 0 0 0 1	
2.944E-02	8.310E+00	ns	F014	0 0 0 0 2	

3333. C₁₄H₁₉Cl₂NO₂

Chlorambucil

N,N-di-(2-Chloroethyl)-γ-(p-aminophenyl)butyric acid

Linfolysin

Elcoril

Linfolizin

Leukersan

RN: 305-03-3 **MP (°C):** 64**MW:** 304.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	9.127E-02	3	G434	0 0 0 0 0	pH 4.13
<3.29E-03	<1.00E+00	30	L343	2 1 1 1 0	EFG

3334. C₁₄H₁₉IN₂O₆

Uridine, 2'-deoxy-5-iodo-, 5'-pentanoate

5'-Valeryl 5-iodo-2'-deoxyuridine

RN: 84052-69-7 **MP (°C):** 142.5**MW:** 438.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E+02	1.753E+05	25	N332	0 0 0 0 0	pH 7.4

3335. C₁₄H₁₉IN₂O₆

Uridine, 2'-deoxy-5-iodo-, 5'-(2,2-dimethylpropanoate)

5'-Pivaloyl 5-iodo-2'-deoxyuridine

5-Iodo-2'-deoxyuridine 5'-pivalate

RN: 84043-28-7 **MP (°C):** 106.5**MW:** 438.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.400E+02	1.928E+05	25	N332	0 0 0 0 0	pH 7.4

3336. C₁₄H₁₉NO

n-Pentylcinnamamide

2-Propenamide, N-pentyl-3-phenyl-

RN: 23784-51-2 **MP (°C):****MW:** 217.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	1.782E-02	ns	H350	0 0 0 0 0	

3337. C₁₄H₁₉NO₃

Acetaminophen hexanoate

Hexanyl acetaminophen

Hexanoic acid, 4-(acetylamino)phenyl ester

4'-Hydroxyacetanilide hexanoate

RN: 20675-21-2 MP (°C): 107

MW: 249.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.220E-05	1.800E-02	25	B010	1 1 1 1 0	
2.286E-04	5.700E-02	37	D029	0 0 0 0 0	

3338. C₁₄H₁₉NO₃

Propanamide, 2-(benzoyloxy)-N,N-diethyl-

RN: 115178-79-5 MP (°C): 53.5

MW: 249.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.214E-03	1.300E+00	22	N317	1 1 2 1 2	

3339. C₁₄H₁₉NO₄

Anisomycin

(2R,3R,4R)-2-(4-Methoxybenzyl)-3,4-pyrrolidinediol-3-acetate

RN: 22862-76-6 MP (°C): 140.5

MW: 265.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.469E-02	6.550E+00	28	A038	2 0 1 1 2	

3340. C₁₄H₁₉N₃S

Methapyrilene

N,N-Dimethyl-N',2-pyridinyl-N'-(2-thienylmethyl)-1,2-ethanediamine

Cope

A 3322

AH-42

Semiken

RN: 91-80-5 MP (°C): <25

MW: 261.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	6.012E-01	30	L068	1 0 0 1 0	EFG
1.700E-02	4.444E+00	37.5	L034	2 2 0 1 2	pH 7.4

3341. C₁₄H₁₉N₃S

Thenyldiamine

1,2-Ethanediamine, *N,N*-dimethyl-*N'*-2-pyridinyl-*N'*-(3-thienylmethyl)-
N-(2-Dimethylaminoethyl)-*N*-2-pyridyl-3-thenylamine

Thefanil

Thenfadil

Tenfidil

RN: 91-79-2**MP (°C):****MW:** 261.39**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	4.444E+00	37.5	L034	2 2 0 1 2	pH 7.4

3342. C₁₄H₁₉N₅O₄

N,N-Diethylsuccinamyloxymethyl-1-allopurinol

Butanoic acid, 4-(diethylamino)-4-oxo-, (4,5-dihydro-4-oxo-1*H*-pyrazolo[3,4-d]pyrimidin-1-yl)
methyl ester**RN:** 98827-27-1 **MP (°C):** 138-140**MW:** 321.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.027E-01	3.300E+01	22	B322	0 0 0 0 0	

3343. C₁₄H₁₉N₅O₅9-[5'-(*O*-Butyryl)-β-D-arabinofuranosyl]adenine ester

Vidarabine 5'-butyrate

RN: 65926-30-9 **MP (°C):****MW:** 337.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.773E-02	1.610E+01	ns	B134	0 1 1 1 2	

3344. C₁₄H₁₉O₆P

Crotoxyphos

Dimethylphosphate of α-methylbenzyl-3-hydroxy-*cis*-crotonate**RN:** 7700-17-6 **MP (°C):****MW:** 314.28 **BP (°C):** 135

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.179E-03	9.990E-01	ns	M061	0 0 0 0 0	
3.182E-03	1.000E+00	rt	M161	0 0 0 0 0	

3345. C₁₄H₂₀ClNO₂

Alachlor

2-Chloro-2',6'-diethyl-N-(methoxymethyl)acetanilide

RN: 15972-60-8 MP (°C): 39.5

MW: 269.77 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.896E-04	2.400E-01	23	M161	1 0 0 0 2	
5.486E-04	1.480E-01	25	B200	1 0 0 0 2	
5.486E-04	1.480E-01	ns	M061	0 0 0 0 2	
5.560E-04	1.500E-01	ns	M110	0 0 0 0 0	
8.896E-04	2.400E-01	ns	V414	0 0 0 0 0	EFG

3346. C₁₄H₂₀ClNO₂

Acetochlor

Doubleplay

Harness

Topnotch

Top Hand

Acenit

RN: 34256-82-1 MP (°C):

MW: 269.77 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.260E-04	2.228E-01	ns	S460	0 0 0 0 0	

3347. C₁₄H₂₀N₂O

Siduron

1-(2-Methylcyclohexyl)-3-phenylurea

RN: 1982-49-6 MP (°C): 133

MW: 232.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.748E-05	1.800E-02	25	B200	1 0 0 0 1	
7.748E-05	1.800E-02	25	G036	1 0 0 0 1	
7.748E-05	1.800E-02	25	M161	1 0 0 0 1	

3348. C₁₄H₂₀N₂O₂

Pindolol

Barbloc

Visken

2-Propanol, 1-(1H-indol-4-yloxy)-3-[(-methylethyl)amino]-

RN: 13523-86-9 **MP (°C):****MW:** 248.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.329E-04	3.300E-02	22.5	B422	2 0 2 2 2	

3349. C₁₄H₂₀N₂O₃S

Tolcyclamide

1-Cyclohexyl-3-*para*-tolylsulfonylurea

Glycyclamide

RN: 664-95-9 **MP (°C):** 175**MW:** 296.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.194E-05	1.836E-02	37	A028	1 0 2 1 2	
6.200E-05	1.838E-02	37	A046	2 0 1 1 2	intrinsic

3350. C₁₄H₂₀N₃O₅PS

Pyrazophos

2-[(Diethoxyphosphinothioyl)oxy]-5-methylpyrazolo[1,5-a]pyrimidine-6-carboxylic acid ethyl Ester

Afugan

Curamil

RN: 13457-18-6 **MP (°C):** 50.5**MW:** 373.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.125E-05	4.200E-03	20	A306	0 0 0 0 0	
1.125E-05	4.200E-03	20	M161	1 0 0 0 1	

3351. C₁₄H₂₀N₄O₂

2,5-bis(Methylaziridinyl)-3,6-bis(methylamino)-1,4-benzoquinone

RN: 64947-06-4 **MP (°C):** 179**MW:** 276.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.62E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3352. C₁₄H₂₀N₄O₂

2,5-Diaziridinyl-3,6-bis(dimethylamino)-1,4-benzoquinone

RN: 59886-50-9 MP (°C): 112

MW: 276.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.619E-02	1.000E+01	rt	C317	0 0 0 0 0	

3353. C₁₄H₂₀N₄O₂

2,5-Diaziridinyl-3,6-bis(ethylamino)-1,4-benzoquinone

RN: 59886-53-2 MP (°C): 157

MW: 276.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.809E-03	5.000E-01	rt	C317	0 0 0 0 0	

3354. C₁₄H₂₀N₄O₄

2,5-Diaziridinyl-3,6-bis(hydroxyethylamino)-1,4-benzoquinone

RN: 59886-54-3 MP (°C): 188

MW: 308.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.486E-03	2.000E+00	rt	C317	0 0 0 0 0	

3355. C₁₄H₂₀O₃Heptyl *p*-hydroxybenzoate*n*-Heptyl 4-hydroxybenzoate

RN: 1085-12-7 MP (°C): 48

MW: 236.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.630E-04	6.215E-02	-244	B355	0 0 0 0 0	
2.010E-04	4.750E-02	15	B355	0 0 0 0 0	
2.520E-04	5.955E-02	20	B355	0 0 0 0 0	
5.827E-03	1.377E+00	25	D081	1 2 2 1 2	<i>sic</i>
1.259E-04	2.975E-02	25	F322	2 0 1 1 0	EFG

3356. C₁₄H₂₁NO₂Heptyl *p*-aminobenzoate

Heptyl 4-aminobenzoate

RN: 14309-40-1 MP (°C):

MW: 235.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	4.707E-03	37	F006	1 1 2 2 1	
3.300E-05	7.766E-03	ns	M066	0 0 0 0 1	

3357. C₁₄H₂₁NO₂

2,6-Diisopropyl-4-acetaminophenol

3,5-Diisopropylparacetamol

4-Acetamido-2,6-diisopropylphenol

RN: 1988-14-3 MP (°C):

MW: 235.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.844E-04	1.375E-01	25	D078	1 2 2 1 2	

3358. C₁₄H₂₁NO₂

Octyl nicotinate

Nicotinic acid *n*-octyl ester

RN: 70136-02-6 MP (°C):

MW: 235.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.249E-05	1.000E-02	32	L346	1 0 0 1 2	

3359. C₁₄H₂₁NO₂Benzeneacetamide, *N*-hydroxy- α -dipropyl

RN: 60631-09-6 MP (°C):

MW: 235.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	3.059E-01	26	G076	1 0 0 1	

3360. C₁₄H₂₁NO₂Benzene propanamide, *N*-hydroxy- α 2,4,6-pentamethyl

RN: 60631-10-9 MP (°C):

MW: 235.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	7.060E-02	26	G076	1 0 0 1	

3361. C₁₄H₂₁NO₃

4-Methoxybenzoic acid-2-(diethylamino)ethyl ester

Diethylaminoethyl *p*-anisate

RN: 10367-84-7 MP (°C):

MW: 251.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-03	1.332E+00	ns	M066	0 0 0 0 1	

3362. C₁₄H₂₁NO₄P

Phenyl(di-morpholido)-phosphate

RN: MP (°C):

MW: 298.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.583E+00	7.706E+02	25	A040	1 0 0 0 2	

3363. C₁₄H₂₁N₃O₃

Karbutilate

m-(3,3-Dimethylureido)phenyl-*tert*-butylcarbamate

Tandex

RN: 4849-32-5 MP (°C): 176.3

MW: 279.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.163E-03	3.250E-01	20	B200	1 0 0 0 2	
1.163E-03	3.250E-01	rt	M161	0 0 0 0 2	

3364. C₁₄H₂₁N₃O₃S

Tolazamide

N-((Hexahydro-1H-azepin-1-yl)amino)carbonyl)-4-methylbenzenesulfonamide

Tolinase

N-(*p*-Toluenesulfonyl)-*N'*-hexamethyleniminourea

U 17835

RN: 1156-19-0 MP (°C): 170

MW: 311.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	6.540E-02	30	H025	1 0 2 1 1	
1.124E-03	3.499E-01	ns	B404	0 2 1 1 0	intrinsic

3365. C₁₄H₂₂

2-Octylbenzene

(1-Methylheptyl)benzene

RN: 777-22-0 **MP (°C):**
MW: 190.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.585E-06	3.017E-04	ns	D001	0 0 0 0 2	

3366. C₁₄H₂₂N₂O

Lidocaine

2-(Diethylamino)-N-(2,6-dimethylphenyl)acetamide

2-Diethylamino-2',6'-acetoxylidide

Lignocaine

Leostesin

Xylocaine

RN: 137-58-6 **MP (°C):** 68
MW: 234.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-02	4.335E+00	14.5	N046	2 0 1 1 1	intrinsic
5.460E-05	1.279E-02	22.5	B440	0 0 0 0 0	
1.550E-02	3.632E+00	25	D402	1 2 2 2 0	EFG
1.643E-02	3.850E+00	25	L338	1 0 1 1 2	
1.630E-02	3.820E+00	25	N046	2 0 1 1 1	intrinsic
1.488E-02	3.488E+00	25	S450	0 0 0 0 0	Intrinsic
1.750E-02	4.101E+00	30	L068	1 0 0 1 0	EFG
1.460E-02	3.421E+00	34.5	N046	2 0 1 1 1	intrinsic
1.700E-02	3.984E+00	37	D402	1 2 2 2 0	
1.440E-02	3.375E+00	37	N044	2 1 1 2 2	intrinsic

3367. C₁₄H₂₂N₂O₂

4-Methylaminobenzoic acid-2-(diethyl-amino)ethyl ester

Benzoic acid, 4-(methylamino)-, 2-(diethylamino)ethyl ester

Benzoic acid, *p*-(methylamino)-, 2-(diethylamino)ethyl ester

RN: 16488-52-1 **MP (°C):**
MW: 250.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.750E-03	1.940E+00	ns	M066	0 0 0 0 2	

3368. C₁₄H₂₂N₂O₂

4-Aminobenzoic acid-2-(diethyl-amino)propyl ester
2-Diethylamino)propyl 4-aminobenzoate

RN: 5878-13-7 **MP (°C):**
MW: 250.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-02	3.229E+00	ns	M066	0 0 0 0 2	

3369. C₁₄H₂₂N₂O₃

2,4-Diazaspiro[5.10]hexadecane-1,3,5-trione

RN: 143288-63-5 **MP (°C):**
MW: 266.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-05	6.925E-03	25	P350	0 0 0 0 0	intrinsic

3370. C₁₄H₂₂N₂O₃

Atenolol
Anselol
Apo-atenolol
Benzeneacetamide

4-(2'-Hydroxy-3'-(1-methylethyl)amino)propoxy)-
Noten

RN: 29122-68-7 **MP (°C):**
MW: 266.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.069E-05	1.350E-02	25	A408	2 0 1 2 0	int
7.134E-10	1.900E-07	32	M458	0 0 0 0 0	
9.950E-02	2.650E+01	ns	K444	0 0 0 0 0	

3371. C₁₄H₂₂N₂O₄

Ethyl-2-methyl-2-cyclohexenyl-6-methylmalonurate
Ethyl 2-methyl-2-cyclohexenyl-6-methylmalonurate

RN: **MP (°C):** 97.5
MW: 282.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	2.823E-01	23	B152	1 2 1 1 1	pH 3.5

3372. C₁₄H₂₂N₂O₅

Methoxymethyl-2-methyl-2-cyclohexenyl-6-methylmalonurate

RN: MP (°C): 73

MW: 298.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-03	1.134E+00	23	B152	1 2 1 1 1	pH 3.5

3373. C₁₄H₂₂O

Methyl ionone

6-Methylionone

RN: 1335-46-2 MP (°C):

MW: 206.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.693E-05	2.000E-02	25	M350	1 0 1 1 1	

3374. C₁₄H₂₂O*o-n*-Octylphenol2-*n*-Octylphenol

RN: 949-13-3 MP (°C):

MW: 206.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.385E-05	2.857E-03	25	L022	1 0 0 0 0	

3375. C₁₄H₂₂O*p-n*-Octylphenol

4-Octylphenol

RN: 1806-26-4 MP (°C): 44.5

MW: 206.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.107E-05	1.260E-02	20.5	A335	0 0 0 0 0	
6.120E-05	1.263E-02	20.5	A335	0 0 0 0 0	
8.812E-06	1.818E-03	25	L022	1 0 0 0 0	

3376. C₁₄H₂₃O₃P

Dibutyl phenyl phosphonate
 Dibutoxyphenylphosphine oxide
 Dibutyl phenylphosphonate

RN: 1024-34-6 **MP (°C):**
MW: 270.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.40E-04	<2.00E-01	25	B070	1 2 0 1 0	

3377. C₁₄H₂₄NO₄PS₃

Bensulide
O,O-bis(1-Methylethyl) *S*-(2-((phenylsulfonyl)amino)ethyl) phosphorodithioate
 Betasan
 Betamec
 Exporsan
 Benzulfide

RN: 741-58-2 **MP (°C):** 34.4
MW: 397.52 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.289E-05	2.500E-02	20	B200	1 2 0 0 1	
6.289E-05	2.500E-02	rt	M161	0 0 0 0 1	

3378. C₁₄H₂₄N₂O₃

5-Ethyl-5-*n*-octylbarbituric acid
 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-ethyl-5-octyl-
 5-Ethyl-5-octylbarbiturate

RN: 64810-90-8 **MP (°C):**
MW: 268.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	3.059E-02	25	M310	2 2 2 2 2	

3379. C₁₄H₂₄N₂O₃

p-5-Ethyl-5-methylhexylcarbinylbarbituric acid

RN: **MP (°C):**
MW: 268.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-03	4.140E-01	ns	T003	0 0 0 0 2	

3380. C₁₄H₂₄O₂

3-Hydroxy-2,5-dispirocyclohexyltetrahydrofuran
7-Oxadispiro[5.1.5.2]pentadecan-14-ol

RN: 29839-63-2 **MP (°C):**
MW: 224.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.098E-02	6.951E+00	rt	B066	0 2 0 0 0	contains impurity

3381. C₁₄H₂₆O₄

1,12-Dodecanedicarboxylic acid

Tetradecanedioic acid

RN: 821-38-5 **MP (°C):** 127
MW: 258.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.741E-04	2.000E-01	21	B040	1 0 1 1 0	sic

3382. C₁₄H₂₇NO₂

Pentanamide, N-hydroxy- α,α -dipropyl

RN: **MP (°C):**
MW: 241.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	1.207E-01	26	G076	1 0 0 0 1	

3383. C₁₄H₂₈NO₃PS₂

Piperophos

S-(2-(2-Methyl-1-piperidinyl)-2-oxoethyl) O,O-dipropyl phosphorodithioate

RN: 24151-93-7 **MP (°C):**
MW: 353.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.072E-05	2.500E-02	20	M161	1 0 0 0 1	

3384. C₁₄H₂₈N₂O₂

N,N,N',N'-Tetramethylsebacamide

Decanediamide, N,N,N',N'-tetramethyl-

RN: 13424-83-4 **MP (°C):**
MW: 256.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.270E-01	1.351E+02	30	D010	1 2 1 1 2	

3385. C₁₄H₂₈O₂

Myristic acid

Tetradecanoic acid

Crodacid

1-Tridecanecarboxylic acid

RN: 544-63-8 MP (°C): 54

MW: 228.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.692E-05	1.300E-02	0	B136	1 0 2 1 1	
8.757E-05	2.000E-02	20	B136	1 0 2 1 1	
8.757E-05	2.000E-02	20	D041	1 0 0 0 0	
8.757E-05	2.000E-02	20	R001	1 1 1 1 1	
4.700E-06	1.073E-03	25	J001	1 0 2 1 1	average of 2 intrinsic
8.000E-07	1.827E-04	25	R002	0 0 0 0 0	
3.710E-06	8.473E-04	25	R002	0 0 0 0 0	
9.633E-05	2.200E-02	30	B136	1 0 2 1 1	
1.051E-04	2.400E-02	30	R001	1 1 1 1 1	
1.270E-04	2.900E-02	40	B136	1 0 2 1 1	
1.270E-04	2.900E-02	45	B136	1 0 2 1 1	
1.270E-04	2.900E-02	45	R001	1 1 1 1 1	
1.839E-05	4.200E-03	50	E005	2 1 1 2 1	
9.700E-06	2.215E-03	50	J001	1 0 2 1 1	
1.489E-04	3.400E-02	60	B136	1 0 2 1 1	
2.452E-05	5.600E-03	60	E005	2 1 1 2 1	
1.489E-04	3.400E-02	60	R001	1 1 1 1 1	
5.692E-05	1.300E-02	.0	R001	1 1 1 1 1	

3386. C₁₄H₂₈O₄

1,3-Dioxolane-4-methanol, 2-[2-(heptyloxy)ethyl]-2-methyl

RN: 143458-57-5 MP (°C):

MW: 260.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.440E-03	1.156E+00	25	P342	0 0 0 0 0	0.0001M Na ₂ CO ₃

3387. C₁₄H₂₉NO₂Benzene propanamide, N-hydroxy- α 2,3-pentamethyl

Octanamide, N-hydroxy-2,2-dipropyl

RN: 60631-08-5 MP (°C):

MW: 243.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.095E-01	26	G076	1 0 0 0 1	
1.500E-03	3.651E-01	26	G076	1 0 0 0 1	

3388. C₁₄H₂₉NO₂Octanamide, 2,2,4-triethyl-*N*-hydroxy

RN: 60631-07-4 MP (°C):

MW: 243.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.095E-01	26	G076	1 0 0 0 1	

3389. C₁₄H₂₉NO₂Decanamide, 2,2-diethyl-*N*-hydroxy

RN: 60631-06-3 MP (°C):

MW: 243.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	1.460E-03	26	G076	1 0 0 0 1	

3390. C₁₄H₂₉NO₂Dodecanamide, *N*-hydroxy-2,2-dimethyl

RN: 60631-05-2 MP (°C):

MW: 243.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	3.894E-03	26	G076	1 0 0 0 1	

3391. C₁₄H₂₉NO₂Pentanamide, *N*-hydroxy-4-methyl-2,2-bis(2-methylpropyl)

RN: 60469-53-6 MP (°C):

MW: 243.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E+01	2.434E+03	26	G076	1 0 0 0 1	

3392. C₁₄H₂₉NO₂Hexanamide, 2,2-dibutyl-*N*-hydroxy2,2-Dibutyl-*N*-hydroxyhexanamideTri-*n*-butylacetohydroxamic acid

RN: 52061-82-2 MP (°C):

MW: 243.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	1.704E-02	26	G076	1 0 0 0 1	

3393. C₁₄H₂₉NO₂Tetradecanamide, *N*-hydroxy

Myristohydroxamic acid

N-Hydroxytetradecanamide

RN: 17698-03-2 MP (°C):

MW: 243.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-04	2.434E-02	26	G076	1 0 0 0 1	

3394. C₁₄H₃₀*n*-Tetradecane

Tetradecane

RN: 629-59-4 MP (°C): 5.89

MW: 198.40 BP (°C): 253.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.663E-09	3.300E-07	23	C332	0 0 0 0 0	
3.500E-08	6.944E-06	25	F004	0 0 0 0 0	
1.159E-08	2.300E-06	ns	H123	0 0 0 0 0	

3395. C₁₄H₃₀O

Tetradecanol

RN: 27196-00-5 MP (°C):

MW: 214.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.460E-06	3.130E-04	25	R002	0 0 0 0 0	

3396. C₁₄H₃₀O

Myristyl alcohol

Tetradecanol

RN: 112-72-1 MP (°C): 38

MW: 214.39 BP (°C): 289

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.049E-08	1.940E-05	4	H030	2 2 2 2 2	
9.049E-08	1.940E-05	4	H103	1 2 2 2 2	
8.909E-07	1.910E-04	25	H103	1 2 2 2 2	
5.737E-07	1.230E-04	32	H030	2 2 2 2 2	
5.737E-07	1.230E-04	32	H103	1 2 2 2 2	
1.105E-06	2.370E-04	45	H030	2 2 2 2 2	
1.105E-06	2.370E-04	45	H103	1 2 2 2 2	
2.094E-06	4.490E-04	61	H030	2 2 2 2 2	
2.094E-06	4.490E-04	61	H103	1 2 2 2 2	

3397. C₁₄H₃₁O₂P

Ethyl dihexyl phosphinate

Phosphinic acid, dihexyl-, ethyl ester

RN: 113977-19-8 **MP (°C):****MW:** 262.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.81E-04	<1.00E-01	25	B070	1 2 0 1 0	

3398. C₁₄H₃₁O₃P

Dibutyl hexyl phosphonate

Phosphinic acid, hexyl-, dibutyl ester

RN: 5929-66-8 **MP (°C):****MW:** 278.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<7.18E-04	<2.00E-01	25	B070	1 2 0 1 0	

3399. C₁₄H₃₁O₃P

Diethyl hexyl phosphonate

Phosphinic acid, hexyl-, diethyl ester

RN: 16165-66-5 **MP (°C):****MW:** 278.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.155E-03	6.000E-01	25	B070	1 2 0 1 0	

3400. C₁₄H₃₁O₄P

Dibutyl hexyl phosphate

Phosphoric acid, dibutyl hexyl ester

RN: 80421-90-5 **MP (°C):****MW:** 294.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.40E-04	<1.00E-01	25	B070	1 2 0 1 0	

3401. C₁₄H₃₁O₄P

Diethyl decyl phosphate

Phosphoric acid, decyl ester

RN: 20195-16-8 **MP (°C):****MW:** 294.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.40E-04	<1.00E-01	25	B070	1 2 0 1 0	

3402. C₁₄H₃₁O₅P

Dibutyl ethoxybutyl phosphate

RN: 100888-67-3 MP (°C):

MW: 310.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.255E-03	7.000E-01	25	B070	1 2 0 1 0	

3403. C₁₅H₁₀

4,5-Methylenephenantrene

4H-Cyclopenta[def]phenanthrene

RN: 203-64-5 MP (°C): 76

MW: 190.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.782E-06	1.100E-03	27	D003	1 0 0 1 1	

3404. C₁₅H₁₀Cl₂N₂O₂

Lorazepam

Alzapam

Ativan

Apo-lorazepam

7-Chloro-5-(*o*-chlorophenyl)-1,3-dihydro-3-hydroxy-2H-1,4-benzodiazepin-2-one

RN: 846-49-1 MP (°C): 167

MW: 321.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.681E-04	5.400E-02	ns	N315	0 2 2 1 2	pH 7.09

3405. C₁₅H₁₀O₂

9-Anthracenecarboxylic acid

Anthracene-9-carboxylic acid

RN: 723-62-6 MP (°C): 214

MW: 222.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.824E-04	8.499E-02	24	H106	1 0 2 2 2	
3.825E-07	8.500E-05	ns	M349	0 2 1 1 2	

3406. C₁₅H₁₀O₄S

7-Methylthio-2-xanthonecarboxylic acid

RN: 40363-76-6 MP (°C):

MW: 286.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.081E-07	2.600E-04	25	C059	1 2 1 1 1	

3407. C₁₅H₁₀O₅S

7-Methylsulfinyl-2-xanthonecarboxylic acid

RN: 40691-50-7 MP (°C):

MW: 302.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.064E-06	2.740E-03	25	C059	1 2 1 1 2	

3408. C₁₅H₁₀O₆

Eriodictyol

5,7,3',4'-Tetra-hydroxyflavon

RN: 552-58-9 MP (°C): 257dec

MW: 286.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.445E-04	7.000E-02	20	F300	1 0 0 0 1	
6.987E-04	2.000E-01	100	F300	1 0 0 0 2	

3409. C₁₅H₁₀O₇

Morin

3,5,7,2',4',-Penta-hydroxyflavon

RN: 480-16-0 MP (°C): 299.5

MW: 302.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.271E-04	2.500E-01	20	F300	1 0 0 0 1	
2.978E-03	9.000E-01	100	F300	1 0 0 0 0	

3410. C₁₅H₁₀O₇

Quarceltin

2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one

3,3',4',5,7-Pentahydroxyflavone

3',4',5,7-Tetrahydroxyflavon-3-ol

Xanthaurine

Meletin

RN: 117-39-5 MP (°C): 316–317

MW: 302.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.985E-02	6.000E+00	ns	Z411	0 0 0 0 0	

3411. C₁₅H₁₀O₇.H₂O

Morin hydrate

4H-1-Benzopyran-4-one, 2-(2,4-dihydroxyphenyl)-3,5,7-trihydroxy-, monohydrate

Flavone, 2',3,4',5,7-pentahydroxy-, monohydrate

Morin monohydrate

RN: 6202-27-3 MP (°C):

MW: 320.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.994E-04	1.920E-01	ns	B404	0 2 1 1 0	

3412. C₁₅H₁₁ClF₃NO₄

Oxyfluorfen

Oxyfluorofen

Koltar

Goal

2-Chloro-1-(3-ethoxy-4-nitrophenoxy)-4-(trifluoromethyl)benzene

Goal 1.6E

RN: 42874-03-3 MP (°C): 83–84

MW: 361.71 BP (°C): >240

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.236E-07	1.170E-04	ns	R427	0 0 0 0 0	

3413. C₁₅H₁₁ClN₂O₂

Oxazepam

Serax

7-Chloro-1,3-dihydro-3-hydroxy-5-phenyl-2H-1,4-benzodiazepin-2-one

Apo-oxazepam

Abboxampam

RN: 604-75-1 MP (°C): 205.5

MW: 286.72 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.975E-05	2.000E-02	22	N319	0 0 0 0 0	
1.744E-04	5.000E-02	amb	L434	0 0 0 0 0	
7.673E-05	2.200E-02	c	B362	0 0 0 0 0	

3414. C₁₅H₁₁ClO₃

Chlorflurecol-methyl

Chlorflurenol

Methyl-2-chloro-9-hydroxyfluorene-9-carboxylate

RN: 2536-31-4 MP (°C): 152

MW: 274.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.552E-05	1.800E-02	20	A308	1 0 0 0 1	
7.936E-05	2.180E-02	20	B200	1 0 0 0 2	
6.552E-05	1.800E-02	20	M161	1 0 0 0 1	

3415. C₁₅H₁₁NO₂

C.I. Disperse orange 11

1-Amino-2-methylanthraquinone

2-Methyl-1-anthaquinonylamine

Acetate fast orange R

RN: 82-28-0 MP (°C): 208

MW: 237.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	3.322E-04	25	B333	0 0 0 0 0	

3416. C₁₅H₁₁NO₂

C.I. Disperse red 9

1-(Methylamino)-9,10-anthraquinone

Serilene fast pink BT

Smoke red M

RN: 82-38-2 MP (°C): 161

MW: 237.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-07	7.355E-05	25	B333	0 0 0 0 0	

3417. C₁₅H₁₁NO₃

N-epoxymethyl-1,8-naphthamilide

ENA

RN: MP (°C):

MW: 253.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.580E-05	1.160E-02	ns	D428	0 0 0 0 0	

3418. C₁₅H₁₁N₃

2,2',6,2''-terpyridine

Terpyridine

Triptyridyl

RN: 1148-79-4 MP (°C):

MW: 233.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.310E-03	1.472E+00	24.99	B444	0 0 0 0 0	

3419. C₁₅H₁₁N₃O₃

Nitrazepam

1,3-Dihydro-7-nitro-5-phenyl-2H-1,4-benzodiazepin-2-one

Mogadon

Unisomnia

RN: 146-22-5 MP (°C): 224

MW: 281.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.529E-04	4.300E-02	30	O321	0 0 0 0 0	

3420. C₁₅H₁₂

1-Methylphenanthrene

RN: 832-69-9

MP (°C): 118

MW: 192.26

BP (°C): 358

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.952E-07	9.520E-05	6.60	M063	2 1 2 2 2	
4.950E-07	9.517E-05	6.60	M082	1 1 1 2 2	
4.950E-07	9.517E-05	6.60	M151	2 1 2 2 2	
4.956E-06	9.529E-04	6.64	M183	1 2 1 1 2	
5.929E-07	1.140E-04	8.90	M063	2 1 2 2 2	
5.940E-07	1.142E-04	8.90	M082	1 1 1 2 2	
5.940E-07	1.142E-04	8.90	M151	2 1 2 2 2	
5.933E-07	1.141E-04	8.94	M183	1 2 1 1 2	
7.646E-07	1.470E-04	14.00	M063	2 1 2 2 2	
7.650E-07	1.471E-04	14.00	M082	1 1 1 2 2	
7.650E-07	1.471E-04	14.00	M151	2 1 2 2 2	
7.650E-07	1.471E-04	14.04	M183	1 2 1 1 2	
1.004E-06	1.930E-04	19.20	M063	2 1 2 2 2	
1.010E-06	1.942E-04	19.20	M082	1 1 1 2 2	
1.010E-06	1.942E-04	19.20	M151	2 1 2 2 2	
1.004E-06	1.931E-04	19.24	M183	1 2 1 1 2	
1.326E-06	2.550E-04	24.10	M063	2 1 2 2 2	
1.320E-06	2.538E-04	24.10	M082	1 1 1 2 2	
1.320E-06	2.538E-04	24.10	M151	2 1 2 2 2	
1.327E-06	2.552E-04	24.14	M183	1 2 1 1 2	
1.399E-06	2.690E-04	25.00	M151	2 1 1 2 2	
1.581E-06	3.040E-04	26.90	M063	2 1 2 2 2	
1.580E-06	3.038E-04	26.90	M082	1 1 1 2 2	
1.580E-06	3.038E-04	26.90	M151	2 1 2 2 2	
1.583E-06	3.043E-04	26.94	M183	1 2 1 1 2	
1.846E-06	3.550E-04	29.90	M063	2 1 2 2 2	
1.850E-06	3.557E-04	29.90	M082	1 1 1 2 2	
1.850E-06	3.557E-04	29.90	M151	2 1 2 2 2	
1.848E-06	3.553E-04	29.94	M183	1 2 1 1 2	

3421. C₁₅H₁₂

2-Methylanthracene

RN: 613-12-7

MP (°C): 204

MW: 192.26

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.672E-08	7.060E-06	6.30	M063	2 1 2 2 2	
3.670E-08	7.056E-06	6.30	M082	1 1 1 2 2	
3.670E-08	7.056E-06	6.30	M151	2 1 2 2 2	
3.675E-08	7.066E-06	6.34	M183	1 2 1 1 2	
4.411E-08	8.480E-06	9.10	M063	2 1 2 2 2	
4.410E-08	8.479E-06	9.10	M082	1 1 1 2 2	
4.410E-08	8.479E-06	9.10	M151	2 1 2 2 2	
4.414E-08	8.487E-06	9.14	M183	1 2 1 1 2	

(continued)

3421. C₁₅H₁₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.905E-08	9.430E-06	10.80	M063	2 1 2 2 2	
4.900E-08	9.421E-06	10.80	M082	1 1 1 2 2	
4.900E-08	9.421E-06	10.80	M151	2 1 2 2 2	
4.909E-08	9.438E-06	10.84	M183	1 2 1 1 2	
5.773E-08	1.110E-05	13.90	M063	2 1 2 2 2	
5.750E-08	1.106E-05	13.90	M082	1 1 1 2 2	
5.750E-08	1.106E-05	13.90	M151	2 1 2 2 2	
5.778E-08	1.111E-05	13.94	M183	1 2 1 1 2	
7.542E-08	1.450E-05	18.30	M063	2 1 2 2 2	
7.540E-08	1.450E-05	18.30	M082	1 1 1 2 2	
7.540E-08	1.450E-05	18.30	M151	2 1 2 2 2	
7.550E-08	1.452E-05	18.34	M183	1 2 1 1 2	
9.934E-08	1.910E-05	23.10	M063	2 1 2 2 2	
9.940E-08	1.911E-05	23.10	M082	1 1 1 2 2	
9.940E-08	1.911E-05	23.10	M151	2 1 2 2 2	
9.944E-08	1.912E-05	23.14	M183	1 2 1 1 2	
2.028E-07	3.900E-05	25	M064	1 1 2 2 1	
1.108E-07	2.130E-05	25.00	M151	2 1 1 2 2	
1.259E-07	2.420E-05	27.00	M063	2 1 2 2 2	
1.260E-07	2.423E-05	27.00	M082	1 1 1 2 2	
1.260E-07	2.423E-05	27.00	M151	2 1 2 2 2	
1.260E-07	2.423E-05	27.04	M183	1 2 1 1 2	
1.670E-07	3.210E-05	31.10	M063	2 1 2 2 2	
1.670E-07	3.211E-05	31.10	M082	1 1 1 2 2	
1.670E-07	3.211E-05	31.10	M151	2 1 2 2 2	
1.671E-07	3.213E-05	31.14	M183	1 2 1 1 2	

3422. C₁₅H₁₂

9-Methylanthracene

RN: 779-02-2

MP (°C): 79

MW: 192.26

BP (°C): 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.358E-06	2.610E-04	25	M064	1 1 2 2 2	
1.330E-06	2.557E-04	25	M342	1 0 1 1 2	
1.358E-06	2.610E-04	ns	M344	0 0 0 0 2	

3423. C₁₅H₁₂Cl₂O₃

2,4-Dichlorophenoxyacetic acid benzyl ester

Benzyl 2,4-dichlorophenoxyacetate

2,4-DBE

RN: 13246-97-4 MP (°C):

MW: 311.17 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.955E-05	1.542E-02	ns	M120	0 0 1 1 2	

3424. C₁₅H₁₂Cl₂O₃

Ethanol, 2-(2,4-dichlorophenoxy)-, benzoate
 Benzoate, 2-(2,4-dichlorophenoxy)ethyl-
 2,4-DEB

RN: 94-83-7 **MP (°C):** 74
MW: 311.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-04	4.800E-02	ns	B185	0 0 0 0 0	

3425. C₁₅H₁₂I₃NO₄

Liothyronine
 3,3',5-Triiodothyronine

RN: 6893-02-3 **MP (°C):** 236dec
MW: 650.98 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.080E-06	3.958E-03	37	L094	2 0 0 1 2	pH 4-5, zwitterion

3426. C₁₅H₁₂N₂O

5H-Dibenz[b,f]azepine-5-carboxamide

Carbazepine

5-Carbamoyl-5H-dibenz[b,f]azepine

Iminostilbene

Carbamazepine

Epitol

RN: 298-46-4 **MP (°C):** 190–193

MW: 236.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.655E-04	1.100E-01	20	B196	0 0 0 0 0	
4.700E-04	1.110E-01	20	B196	0 0 0 0 0	
6.349E-04	1.500E-01	25	C437	0 0 0 0 0	Average
1.864E-03	4.404E-01	32	F425	0 0 0 0 0	pH 7.4
1.100E-03	2.600E-01	amb	L434	0 0 0 0 0	
4.232E-05	1.000E-02	ns	K444	0 0 0 0 0	
4.000E-03	9.451E-01	rt	B397	0 0 0 0 0	EFG

3427. C₁₅H₁₂N₂O₂

Phenytoin

5,5-Diphenyl-2,4-imidazolidinedione

Dilantin

5,5-Diphenylhydantoin

Ekko

Zentropil

RN: 57-41-0 MP (°C): 296.5

MW: 252.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.765E-04	9.499E-02	0	B114	1 1 1 2 1	pH 6-7
1.268E-04	3.200E-02	22	B154	1 1 1 1 1	0.1M HCl
7.531E-05	1.900E-02	25	A408	2 0 1 2 0	int
5.549E-05	1.400E-02	25	P061	0 0 0 0 0	pH 1-7
1.526E-04	3.850E-02	37	F183	1 0 1 1 2	intrinsic
2.600E-04	6.559E-02	50	M335	1 0 2 1 2	pH 5
2.323E-04	5.860E-02	ns	K446	0 0 0 0 0	
7.650E-05	1.930E-02	rt	I404	0 0 0 0 0	Average

3428. C₁₅H₁₂N₂O₂

Disperse violet 4

1-Amino-4-(*N*-methylamino)anthraquinone

Interchem acetate violet 6B

RN: 1220-94-6 MP (°C): 193

MW: 252.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-06	5.802E-04	25	B333	0 0 0 0 0	

3429. C₁₅H₁₂N₂O₃5-Phenyl-5-(*p*-hydroxy)phenyl-hydantoinDL-5-(*p*-Hydroxyphenyl)-5-phenylhydantoin*p*-Hydroxyphenytoin

Hydroxydiphenylhydantoin

p-Hydroxydiphenylhydantoin

RN: 2784-27-2 MP (°C):

MW: 268.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.342E-04	3.600E-02	37	F183	1 0 1 1 2	intrinsic

3430. C₁₅H₁₂N₂O₃

Furfurin

1H-Imidazole, 2,4,5-tri-2-furanyl-4,5-dihydro-

2-Imidazoline, 2,4,5-tri-2-furyl-

RN: 550-23-2 **MP (°C):****MW:** 268.27 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.455E-04	2.000E-01	8	F300	1 0 0 0 0	
2.870E-02	7.700E+00	100	F300	1 0 0 0 1	

3431. C₁₅H₁₂O₄Benzoyl-*r*-mandelic acid*p*-Benzoylmandelic acid**RN:** 100915-04-6 **MP (°C):** 177**MW:** 256.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.980E-02	5.074E+00	0	A043	1 2 1 1 1	
1.980E-02	5.074E+00	0	L035	1 2 2 1 1	
2.327E-02	5.964E+00	10	A043	1 2 1 1 1	
2.327E-02	5.964E+00	10	L035	1 2 2 1 1	
2.520E-02	6.458E+00	15	A043	1 2 1 1 1	
2.520E-02	6.458E+00	15	L035	1 2 2 1 1	
2.828E-02	7.247E+00	20	A043	1 2 1 1 1	
2.828E-02	7.247E+00	20	L035	1 2 2 1 1	
3.059E-02	7.838E+00	25	A043	1 2 1 1 1	
3.059E-02	7.838E+00	25	L035	1 2 2 1 1	
3.557E-02	9.116E+00	30	A043	1 2 1 1 1	
3.557E-02	9.116E+00	30	L035	1 2 2 1 1	
4.017E-02	1.029E+01	35	A043	1 2 1 1 2	
4.017E-02	1.029E+01	35	L035	1 2 2 1 2	
4.894E-02	1.254E+01	40	A043	1 2 1 1 2	
4.894E-02	1.254E+01	40	L035	1 2 2 1 2	
6.032E-02	1.546E+01	45	A043	1 2 1 1 2	
6.032E-02	1.546E+01	45	L035	1 2 2 1 2	
7.201E-02	1.845E+01	50	A043	1 2 1 1 2	
7.201E-02	1.845E+01	50	L035	1 2 2 1 2	

3432. C₁₅H₁₂O₄

Benzoic acid, 2-(acetoxy)-, phenyl ester

Phennin

Phenyl 2-acetoxybenzoate

Vesipyrin

Spiroform

Phenyl acetylsalicylate

RN: 134-55-4 MP (°C): 97.5

MW: 256.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.805E-05	2.000E-02	21	N335	0 0 0 0 0	

3433. C₁₅H₁₃Cl₃O₂

2-p-Methoxyphenyl-2-p-hydroxyphenyl-1,1,1-trichloro-ethane

Phenol, 4-[2,2,2-trichloro-1-(4-methoxyphenyl)ethyl]-

RN: 28463-03-8 MP (°C): 112–114

MW: 331.63 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.412E-06	8.000E-04	ns	K117	0 1 2 1 1	

3434. C₁₅H₁₃FO₂

Flurbiprofen

3-Fluoro-4-phenylhydratropic acid

Froben

Ansaid

RN: 5104-49-4 MP (°C): 110

MW: 244.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-05	6.180E-03	5	F306	1 0 1 2 2	intrinsic
2.761E-05	6.744E-03	24.99	K447	0 0 0 0 0	pH 2.0
4.339E-05	1.060E-02	25	A408	2 0 1 2 0	int
5.000E-05	1.221E-02	25	A411	1 0 0 1 0	int
1.332E-04	3.254E-02	25	C314	0 0 0 0 0	
1.331E-04	3.250E-02	25	C314	0 0 0 0 0	
3.870E-05	9.453E-03	25	F306	1 0 1 2 2	intrinsic
1.940E-04	4.739E-02	25	O303	1 0 0 1 0	EFG
4.600E-05	1.124E-02	37	F306	1 0 1 2 2	intrinsic
2.866E-05	7.000E-03	37	Y421	0 0 0 0 0	
>2.05E-03	>5.00E-01	ns	B404	0 2 1 1 0	
2.700E-04	6.595E-02	ns	O304	0 0 1 2 2	
3.275E-05	8.000E-03	rt	H302	0 0 2 1 2	intrinsic

3435. C₁₅H₁₃F₃N₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-methyl-4-(trifluoromethyl)-

RN: 135794-72-8 **MP (°C):**
MW: 322.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.209E-05	2.001E-02	ns	M381	0 1 1 1 2	pH 7.0

3436. C₁₅H₁₃NO

7-Benzoylindoline

U-26,952

RN: 33244-57-4 **MP (°C):** 124
MW: 223.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.026E-05	2.290E-03	25	C046	0 0 0 0 0	

3437. C₁₅H₁₃NO₂

Dibenz[b,f][1,4]oxazepin-11(10H)-one, 10-ethyl-

RN: 17296-50-3 **MP (°C):**
MW: 239.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.089E-04	4.999E-02	ns	M381	0 1 1 1 2	pH 7.0

3438. C₁₅H₁₃NO₂S

Metiazinic acid

Methiazinic acid

RN: 13993-65-2 **MP (°C):** 146
MW: 271.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.142E-04	3.100E-02	30	D015	2 0 1 1 0	EFG
2.211E-04	6.000E-02	37	D015	2 0 1 1 0	EFG

3439. C₁₅H₁₃NO₃

Ketorolac

RN: 74103-06-3 **MP (°C):**
MW: 255.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.167E-04	1.830E-01	32	C411	2 1 1 2 1	
4.309E-04	1.100E-01	37	Y421	0 0 0 0 0	

3440. C₁₅H₁₃NO₃

Benzoyl acetaminophen

Acetamide, N-[4-(benzoyloxy)phenyl]-

Acetanilide, 4'-hydroxy-, benzoate (ester)

RN: 537-52-0 MP (°C): 170.5–171.5

MW: 255.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.659E-05	1.700E-02	37	D029	0 0 0 0 0	

3441. C₁₅H₁₃NO₄

Phenyl acetaminophen

Carbonic acid, 4-(acetylamino)phenyl phenyl ester

Acetanilide, 4'-hydroxy-, phenyl carbonate (ester)

RN: 17239-23-5 MP (°C): 139–140.5

MW: 271.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.322E-04	6.300E-02	37	D029	0 0 0 0 0	

3442. C₁₅H₁₃N₃O₄S

Piroxicam

2H-1,2-Benzothiazine-3-carboxamide, 4-hydroxy-2-methyl-N-2-pyridinyl-, 1,1-dioxide

Fensaid

Feldene

Candyl

Mobilis

RN: 36322-90-4 MP (°C): 198

MW: 331.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.535E-04	8.400E-02	25	M457	0 0 0 0 0	
1.608E-04	5.330E-02	32	C411	2 1 1 2 1	
<3.02E-04	<1.00E-01	rt	B435	0 0 0 0 0	
6.941E-05	2.300E-02	rt	H302	0 0 2 1 2	intrinsic

3443. C₁₅H₁₄ClN₃O₄S

Cefaclor

5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[(2*R*)-aminophenylacetyl]amino]-3-chloro-8-oxo-, (6*R*,7*R*)-

Ceclor

Alfacet

Cephaclor

RN: 53994-73-3 **MP (°C):**
MW: 367.81 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.719E-02	1.000E+01	ns	L099	0 0 0 0 0	

3444. C₁₅H₁₄ClN₃O₄S₃

Benzthiazide

Exna

Hydrex

RN: 91-33-8 **MP (°C):**
MW: 431.94 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.547E-05	1.100E-02	ns	B404	0 2 1 1 0	
6.482E-06	2.800E-03	rt	I404	0 0 0 0 0	Intrinsic, Average

3445. C₁₅H₁₄Cl₂F₃N₃O₃

Carfentrazone-ethyl

Df herbicide

Benzene propanoic acid, α-2-dichloro-5-{4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl}-4-fluoro-, ethyl ester

Ethyl 2-chloro-3-{2-chloro-4-fluoro-5-{4-(difluoromethyl)-4,5-dihydro-3-methyl-5-oxo-1H-1,2,4-triazol-1-yl}phenyl}propanoate

F 8426

RN: 128639-02-1 **MP (°C):**
MW: 412.20 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.333E-05	2.198E-02	ns	S460	0 0 0 0 0	

3446. C₁₅H₁₄Cl₂N₄O₃

C.I. Disperse orange 5

Ethanol, 2-[[4-[(2,6-dichloro-4-nitrophenyl)azo]phenyl]methylamino]

Amacel fast brown 3R

Celliton fast brown 3R

RN: 6232-56-0 **MP (°C):** 127**MW:** 369.21 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-07	1.588E-04	25	B333	0 0 0 0 0	
8.938E-06	3.300E-03	60	P313	0 0 0 0 0	average of 2
1.530E-05	5.650E-03	70	P313	0 0 0 0 0	average of 2
2.939E-05	1.085E-02	80	P313	0 0 0 0 0	average of 2
6.378E-05	2.355E-02	90	P313	0 0 0 0 0	average of 2
1.354E-04	5.000E-02	100	P313	0 0 0 0 0	average of 2

3447. C₁₅H₁₄F₃N₃O₄S₂

Bendroflumethiazide

Corzide

Rauzide

Naturetin

RN: 73-48-3 **MP (°C):** 222**MW:** 421.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-04	5.057E-02	20	A080	1 0 2 1 2	
2.570E-04	1.083E-01	25	A076	1 0 1 1 2	
2.847E-05	1.200E-02	ns	B404	0 2 1 1 0	
9.492E-05	4.000E-02	rt	A095	0 0 2 2 0	
3.631E-05	1.530E-02	rt	I404	0 0 0 0 0	Intrinsic, Average

3448. C₁₅H₁₄NO₂PS

Cyanofenphos

O-(4-Cyanophenyl) O-ethyl phenylphosphonothioate

Surecide

RN: 13067-93-1 **MP (°C):** 83**MW:** 303.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.978E-06	6.000E-04	30	M161	1 0 0 0 0	

3449. C₁₅H₁₄N₂O₂

Dibenz[b,f][1,4]oxazepin-11(10H)-one, 8-amino-2-methyl-

RN: 155206-47-6 **MP (°C):****MW:** 254.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-04	3.001E-02	ns	M381	0 1 1 1 2	pH 7.0

3450. C₁₅H₁₄N₂O₃*p*-(3-Phenylureido)phenyl acetate

Benzeneacetic acid, 4-[[[phenylamino)carbonyl]amino]-

RN: 181518-40-1 **MP (°C):****MW:** 270.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-05	9.730E-03	25	A066	1 0 1 1 1	

3451. C₁₅H₁₄N₂O₅

2'-Ethoxy-2hydroxy-5-nitrobenzalide

Benzamide, *N*-(2-ethoxyphenyl)-2-hydroxy-5-nitro-**RN:** 213460-67-4 **MP (°C):****MW:** 302.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.687E-05	5.098E-03	25	D400	2 0 0 1 2	

3452. C₁₅H₁₄N₂O₅

4'-Ethoxy-2-hydroxy-3-nitrobenzalide

Benzamide, *N*-(4-ethoxyphenyl)-2-hydroxy-3-nitro-**RN:** 213460-61-8 **MP (°C):****MW:** 302.29 **BP (°C):** 342.2–426.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.119E-05	9.428E-03	25	D400	2 0 0 1 2	

3453. C₁₅H₁₄N₂O₅

2'-Ethoxy-2-hydroxy-3-nitrobenzalide

Benzamide, *N*-(2-ethoxyphenyl)-2-hydroxy-3-nitro-**RN:** 213460-63-0 **MP (°C):****MW:** 302.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.432E-05	7.352E-03	25	D400	2 0 0 1 2	

3454. C₁₅H₁₄N₄O

Nevarapine

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-cyclopropyl-5,11-dihydro-4-methyl

Nevirapine

BI-RG 587

RN: 129618-40-2 **MP (°C):** 248**MW:** 266.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.755E-04	1.000E-01	ns	K444	0 0 0 0 0	
6.412E-04	1.708E-01	ns	M381	0 1 1 1 2	pH 7.0

3455. C₁₅H₁₄O₃

Methyl benzoyl benzoate

Benzoic acid, 4-hydroxy-, (4-methylphenyl)methyl ester

RN: 84833-58-9 **MP (°C):****MW:** 242.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.064E-04	5.000E-02	ns	F014	0 0 0 0 0	

3456. C₁₅H₁₄O₃

[4-(Benzoyloxy)phenyl]acetic acid

(4-Boph)

RN: 6547-53-1 **MP (°C):****MW:** 242.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.711E-04	6.568E-02	20	K437	0 0 0 0 0	pH 2.0
3.711E-04	8.990E-02	25	K437	0 0 0 0 0	pH 2.0
6.338E-04	1.536E-01	30	K437	0 0 0 0 0	pH 2.0
7.293E-04	1.767E-01	37	K437	0 0 0 0 0	pH 2.0

3457. C₁₅H₁₄O₃

Fenoprofen

Fenoporfén

Progesic

Fenpron

Nalfon

Fenopron

RN: 31879-05-7 **MP (°C):****MW:** 242.28 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-04	1.000E-01	37	Y421	0 0 0 0 0	

3458. C₁₅H₁₅ClF₃N₃O

Triflumizole

RN: 99387-89-0 MP (°C): 63.5

MW: 345.75 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.480E-05	1.549E-02	25	V410	0 0 0 0 0	

3459. C₁₅H₁₅ClN₂O₂

Chlorooxuron

(N'-4-(4-Chlorophenoxy)phenyl-N,N-dimethylurea)

3-[p-(p'-Chlorophenoxy)phenyl]-1,1-dimethylurea

N-4-(4'-Chlorophenoxy)phenyl-N',N'-dimethylurea

Tenoran

RN: 1982-47-4 MP (°C): 151

MW: 290.75 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.273E-05	3.700E-03	20	B185	0 0 0 0 0	
1.273E-05	3.700E-03	20	G036	1 0 0 0 1	
1.273E-05	3.700E-03	20	M161	1 0 0 0 1	pH 7
9.286E-06	2.700E-03	ns	B200	0 0 0 0 1	
1.273E-04	3.700E-02	ns	M061	0 0 0 0 1	

3460. C₁₅H₁₅ClN₂O₄S

Xipamide

2',6'-Salicyloxylidide, 4-chloro-5-sulfamoyl-

Aquaphor

Aquaphor (diuretic)

BEI 1293

Diurex

RN: 14293-44-8 MP (°C): 256

MW: 354.81 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.635E-04	5.800E-02	25	H074	1 2 2 1 1	

3461. C₁₅H₁₅CIN₄O₆S

Chlorimuron-ethyl

Chlorimuron ethyl ester

Classic 75DF

Classic

Chlorimuron Et

2-[[[[(4-Chloro-6-methoxy-2-pyrimidinyl)amino]carbonyl]amino]sulfonyl]benzoic acid ethyl ester

RN: 90982-32-4 **MP (°C):** 180–182**MW:** 414.83 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.455E-06	1.018E-03	ns	R427	0 0 0 0 0	

3462. C₁₅H₁₅ClO

2-Benzyl-3,5-dimethyl-4-chloro-phenol

RN: 1867-85-2 **MP (°C):****MW:** 246.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.234E-02	25	B316	0 0 0 0 0	

3463. C₁₅H₁₅NO₂

Mefenamic acid

2',3'-Dimethyl-N-phenyl-anthranilic acid

Forte mefenamic acid

N-(2,3-Xylyl)anthranilic acid

Ponstel

Ponstan

RN: 61-68-7 **MP (°C):** 230.5**MW:** 241.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.289E-05	2.000E-02	30	D015	2 0 1 1 0	EFG
2.800E-05	6.756E-03	35	H091	1 2 2 2 1	<i>sic</i>
1.658E-04	4.000E-02	37	D015	2 0 1 1 0	EFG
1.658E-06	4.000E-04	37	P432	0 0 0 0 0	
1.227E-04	2.960E-02	37	P432	0 0 0 0 0	
8.289E-07	2.000E-04	37	Y421	0 0 0 0 0	
1.100E-04	2.654E-02	ns	O304	0 0 1 2 2	

3464. C₁₅H₁₅NO₃

Tolmetin

Tolectin

RN: 26171-23-3 **MP (°C):**
MW: 257.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.773E-05	2.000E-02	37	Y421	0 0 0 0 0	

3465. C₁₅H₁₅N₃O

5H-Pyrido[2,3-b][1,5]benzodiazepine-5-one, 11-ethyl-6,11-dihydro-6-methyl-

RN: 132686-75-0 **MP (°C):**
MW: 253.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.782E-05	4.515E-03	ns	M381	0 1 1 1 2	pH 7.0
4.742E-04	1.201E-01	ns	M381	0 1 1 1 2	pH 7.0

3466. C₁₅H₁₅N₃O₂

Pyrido[2,3-b][1,5]benzoxazepin-5(6H)-one, 3-amino-6,7,9-trimethyl-

RN: **MP (°C):**
MW: 269.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.730E-04	4.658E-02	ns	M381	0 1 1 1 2	pH 7.0

3467. C₁₅H₁₅N₃O₂

C.I. Disperse yellow 3

Acetamide, N-[4-[(2-hydroxy-5-methylphenyl)azo]phenyl]-

RN: 2832-40-8 **MP (°C):** 195
MW: 269.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-07	3.232E-05	25	B333	0 0 0 0 0	

3468. C₁₅H₁₅N₃S

5H-Pyrido[2,3-b][1,5]benzodiazepine-5-thione, 11-ethyl-6,11-dihydro-6-methyl-

RN: 132686-95-4 **MP (°C):**
MW: 269.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.968E-05	5.301E-03	ns	M381	0 1 1 1 2	pH 7.0

3469. C₁₅H₁₆N₂O₂

Ancymidol

α-Cyclopropyl-α-(4-methoxyphenyl)-5-pyrimidinemethanol

A-Rest

RN: 12771-68-5 MP (°C): 110.5

MW: 256.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.536E-03	6.500E-01	25	M161	1 0 0 0 2	

3470. C₁₅H₁₆N₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 5,11-dihydro-5-methyl-11-propyl-

RN: 132312-81-3 MP (°C):

MW: 268.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.327E-03	3.562E-01	ns	M381	0 1 1 1 2	pH 7.0

3471. C₁₅H₁₆N₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2,4-dimethyl-

RN: 134698-31-0 MP (°C):

MW: 268.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.793E-05	7.493E-03	ns	M381	0 1 1 1 2	pH 7.0

3472. C₁₅H₁₆N₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 5,11-diethyl-5,11-dihydro-

RN: 132312-82-4 MP (°C):

MW: 268.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-03	3.704E-01	ns	M381	0 1 1 1 2	pH 7.0

3473. C₁₅H₁₆N₄O₂

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-methoxy-4-methyl-

RN: 135794-75-1 MP (°C):

MW: 284.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.031E-06	1.999E-03	ns	M381	0 1 1 1 2	pH 7.0

3474. C₁₅H₁₆N₄O₂

1H-Purine-2,6-dione, 1,3-diethyl-3,7-dihydro-8-phenyl-

1,3-Diethyl-8-phenylxanthine

8-Phenyl-1,3-diethylxanthine

RN: 75922-48-4 **MP (°C):****MW:** 284.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.517E-06	1.000E-03	ns	H316	0 0 0 0 0	0.1N HCL
2.110E-05	6.000E-03	ns	H316	0 0 0 0 0	pH 7.4

3475. C₁₅H₁₆N₄O₅S

Benzenesulfonic acid, 4-(1,3-Diethyl-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl)-

RN: 89073-47-2 **MP (°C):** >360**MW:** 364.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.56E-01	>5.70E+01	ns	H316	0 0 0 0 0	pH 7.4
>2.20E-02	>8.00E+00	ns	H316	0 0 0 0 0	0.1N HCL

3476. C₁₅H₁₆O₂

Bisphenol A

2,2-*bis*-[4-Hydroxyphenyl]-propan2,2-*bis*-(4-Hydroxyphenyl)-propane**RN:** 80-05-7 **MP (°C):****MW:** 228.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.533E-03	3.500E-01	20	F300	1 0 0 0 1	
4.775E-04	1.090E-01	22	Y419	0 0 0 0 0	
1.314E-03	3.000E-01	23	S448	0 0 0 0 0	*Temperature 20-25
5.256E-04	1.200E-01	23	S448	0 0 0 0 0	*Temperature 20-25
5.256E-04	1.200E-01	25	D415	1 0 0 0 0	
5.256E-04	1.200E-01	25	D416	0 0 0 0 0	
1.314E-03	3.000E-01	25	S468	0 0 0 0 0	

3477. C₁₅H₁₆O₂

Bisphenol A

RN: 80-05-7

MP (°C):

MW: 228.29

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.256E-04	1.200E-01	25	D416	0 0 0 0 0	

3478. C₁₅H₁₆O₂

Nabumetone

RN: 42924-53-8

MP (°C):

MW: 228.29

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.628E-05	6.000E-03	22.5	C438	0 0 0 0 0	

3479. C₁₅H₁₆O₃

Osthole

2H-1-Benzopyran-2-one, 7-methoxy-8-(3-methyl-2-butenyl)-

RN: 484-12-8 MP (°C): 83.5

MW: 244.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.912E-05	1.200E-02	30	B144	1 0 1 0 1	

3480. C₁₅H₁₆O₉.2H₂O

Aesculin (dihydrate)

Esculin

6,7-Dihydroxycoumarin 6-glucoside

2H-1-Benzopyran-2-one, 6-(β-D-glucopyranosyloxy)-7-hydroxy-

RN: 531-75-9 MP (°C): 205dec

MW: 376.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.605E-03	1.733E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3481. C₁₅H₁₇FN₄O₂

Flupirtine

Carbamic acid, [2-amino-6-[(4-fluorophenyl)methyl]amino]-3-pyridinyl-, ethyl ester

RN: 56995-20-1 MP (°C): 175.8–177.7

MW: 304.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.286E-03	1.000E+00	ns	D321	0 0 0 0 0	

3482. C₁₅H₁₇NO₃

Acetamide, 2-(benzoyloxy)-N,N-di-acetamide, 2-(benzoyloxy)-N,N-di-2-propenyl-

RN: 106231-58-7 MP (°C): 42.5

MW: 259.31 BP (°C): 401.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.738E-03	7.100E-01	22	B427	1 0 0 1 1	in 0.01M HCl
2.738E-03	7.100E-01	22	N317	1 1 2 1 2	

3483. C₁₅H₁₇NO₅

L-Proline, 1-[(benzoyloxy)acetyl]-, methyl ester

RN: 115178-76-2 MP (°C): 72.5

MW: 291.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.239E-03	2.400E+00	22	N317	1 1 2 1 2	

3484. C₁₅H₁₇NO₇

Glycine, N-[[[2-(acetyloxy)benzoyl]oxy]acetyl]-, ethyl ester

RN: 118247-03-3 MP (°C): 68.5

MW: 323.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-02	4.320E+00	21	N335	0 0 0 0 0	

3485. C₁₅H₁₇N₃O₃S

L-Ala-dapsone

2-Amino-N-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)-propanamide

RN: 160348-99-2 MP (°C):

MW: 319.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.066E-02	6.600E+00	25	P351	0 0 0 0 0	pH 7.4
>9.39E-02	>3.00E+01	25	P351	0 0 0 0 0	

3486. C₁₅H₁₈Cl₂N₂O₃

Oxadiazon

3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-one

Ronstar

Scotts OH I

RP-17623

RN: 19666-30-9 MP (°C): 88

MW: 345.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.028E-06	7.000E-04	20	M161	1 0 0 0 0	
2.028E-06	7.000E-04	24	C105	2 1 2 2 2	

3487. C₁₅H₁₈I₃NO₅

Iopronic acid

Butanoic acid, 2-[[2-[3-(acetylamino)-2,4,6-triiodophenoxy]ethoxy]methyl]-

RN: 37723-78-7 MP (°C): 130

MW: 673.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.984E-02	2.008E+01	37	J016	1 0 0 0 2	pH 7.4
1.456E-04	9.799E-02	50	F013	1 0 1 1 1	

3488. C₁₅H₁₈N₂O₃

N-Acetyl-L-tryptophan ethyl ester

RN: 2382-80-1 MP (°C): 106

MW: 274.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.896E-03	5.200E-01	5	L081	2 2 2 2 1	
5.359E-03	1.470E+00	28	L081	2 1 2 2 2	

3489. C₁₅H₁₈N₄O₃S

2-(N4-Acetylulfanilylamo)-4-ethyl-5-methylpyrimidine

RN: **MP (°C):**
MW: 334.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.077E-05	3.600E-03	37	R076	1 2 0 0 1	

3490. C₁₅H₁₈N₄O₃S

2-(N4-Acetylulfanilylamo)-4-n-propylpyrimidine

RN: **MP (°C):**
MW: 334.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.914E-05	6.400E-03	37	R076	1 2 0 0 2	

3491. C₁₅H₁₈N₄O₅

Mitomycin C

MMC

6-Amino-8-[[aminocarbonyl]oxy]methyl]-1,1α,2,8,8α,8β-hexahydro-8α-methoxy-5-methyl,[1aS-(1α,8β,8α,8bα)]-azirino[2',3':3,4]pyrrolo[1,2a]indole-4,7-dione

Mitomycinum

RN: 50-07-7 **MP (°C):** >360
MW: 334.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.730E-03	9.127E-01	25	M316	1 1 1 1 2	
8.500E-01	2.842E+02	ns	B406	0 0 2 2 0	EFG

3492. C₁₅H₁₈O₃

Santonin

Naphtho[1,2-b]furan-2,8(3H,4H)-dione, 3α,5,5α,9β-tetrahydro-3,5α,9-trimethyl-, (3S,3αS,5αS,9βS)-

RN: 481-06-1 **MP (°C):** 170
MW: 246.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.120E-04	2.000E-01	17.5	F300	1 0 0 0 0	
1.624E-02	4.000E+00	100	F300	1 0 0 0 0	

3493. C₁₅H₁₈O₄ β -Cyclopentylpropionyl salicylate

RN: MP (°C):
MW: 262.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.060E-04	2.780E-02	25.6	G015	1 0 1 1 2	pH 1.00, pka 3.91, intrinsic

3494. C₁₅H₁₉ClO₂1,1-Dichloro-1-methyl-2,2-bis(*p*-methoxylphenyl)ethane

RN: 56288-27-8 **MP (°C):**
MW: 266.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.373E-06	1.700E-03	rt	C122	0 0 0 0 0	

3495. C₁₅H₁₉NO*N,N*-HexamethylenecinnamamideHexahydro-1-(1-oxo-3-phenyl-2-propenyl)1*H*-azepine

RN: 59832-05-2 **MP (°C):**
MW: 229.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E-04	5.641E-02	ns	H350	0 0 0 0 0	

3496. C₁₅H₁₉NO*N*-Cyclohexylcinnamamide2-Propenamide, *N*-cyclohexyl-3-phenyl-

RN: 6750-98-7 **MP (°C):**
MW: 229.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.040E-05	9.265E-03	ns	H350	0 0 0 0 0	

3497. C₁₅H₁₉NO₂

Tropacocaine

RN: 537-26-8

MP (°C): 49

MW: 245.32

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	1.055E+00	15	K059	2 2 2 0 1	

3498. C₁₅H₁₉NO₃

1H-Azepine, 1-[(benzoyloxy)acetyl]hexahydro-

RN: 115178-68-2 MP (°C): 107.5

MW: 261.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.870E-03	7.500E-01	22	N317	1 1 2 1 2	

3499. C₁₅H₁₉NO₅

Benzoic acid, 2-(acetoxy)-, 2-(diethylamino)-2-oxoethyl ester

RN: 116482-56-5 MP (°C): 76.5

MW: 293.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.773E-03	2.280E+00	21	N335	0 0 0 0 0	

3500. C₁₅H₂₀N₂O₄

Benzyl-2,2-diethylmalonurate

Benzyl 2,2-diethylmalonurate

RN: 73632-78-7 MP (°C): 107

MW: 292.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-04	6.431E-02	23	B152	1 2 1 1 1	pH 3.5

3501. C₁₅H₂₀N₂O₄S

Acetohexamide

Acetohexamid

1-(*p*-Acetylbenzenesulfonyl)-3-cyclohexylurea

Dymelor

Dimelin

RN: 968-81-0 **MP (°C):** 189
MW: 324.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.706E-04	2.500E-01	25	K023	1 0 2 2 1	EFG, pH 6.5, average of 2
3.483E-05	1.130E-02	37	B130	1 2 1 1 2	pH 1.5, form II
4.963E-05	1.610E-02	37	B130	1 2 1 1 2	pH 1.5, form III
8.015E-05	2.600E-02	37	K106	1 2 2 2 0	EFG, form I
9.556E-05	3.100E-02	37	K106	1 2 2 2 0	EFG, form II

3502. C₁₅H₂₀N₄O₂S

2-Sulfanilylamino-4-amylpyrimidine

RN: 107203-72-5 **MP (°C):**
MW: 320.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.242E-04	2.000E-01	37	R076	1 2 0 0 1	

3503. C₁₅H₂₀N₄O₅

1,5-Dibutyryloxymethyl allopurinol

RN: 98827-19-1 **MP (°C):** 122–123
MW: 336.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.487E-04	5.000E-02	22	B322	0 0 0 0 0	

3504. C₁₅H₂₀N₄O₅

2,5-Dibutyryloxymethyl allopurinol

RN: 98827-20-4 **MP (°C):** 133–135
MW: 336.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.795E-04	9.400E-02	22	B322	0 0 0 0 0	

3505. C₁₅H₂₀N₄O₆9-[5-O-(Butyrate- β -D-arabinofuranosyl)]-6-methoxy-9H-purine

RN: 121032-41-5 MP (°C): 108–110

MW: 352.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.680E-03	3.411E+00	37	M378	1 2 1 1 2	pH 7.2

3506. C₁₅H₂₀N₄O₆.0.3H₂O

2'-Butyryl-6-methoxypurine arabinoside (0.3 hydrate)

RN: 121032-41-5 MP (°C):

MW: 357.75 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.310E-01	8.264E+01	37	C348	0 0 0 0 0	pH 7.00

3507. C₁₅H₂₀N₄O₆

2'-Isobutyryl-6-methoxypurine arabinoside

RN: 121032-44-8 MP (°C):

MW: 352.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-01	2.361E+02	37	C348	0 0 0 0 0	pH 7.00

3508. C₁₅H₂₀N₄O₆.0.25H₂O9-[5-O-(Isobutyrate- β -D-arabinofuranosyl)]-6-methoxy-9H-purine (0.25 hydrate)

RN: 121032-44-8 MP (°C): glass

MW: 356.85 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.830E-02	1.367E+01	37	M378	1 2 1 1 2	pH 7.2

3509. C₁₅H₂₁NO

N,N-Dipropylcinnamamide

Cinnamamide, N,N-dipropyl-

RN: 23784-56-7 MP (°C):

MW: 231.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.890E-03	6.686E-01	ns	H350	0 0 0 0 0	

3510. C₁₅H₂₁NO₂

Meperidine

Ethyl 1-methyl-4-phenylpiperidine-4-carboxylate

Demerol

Dolantin

Pethidine

RN: 57-42-1**MP (°C):** 30**MW:** 247.34**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.648E-02	6.550E+00	25	R338	0 0 0 0 0	
1.300E-02	3.215E+00	30	L068	1 0 0 1 0	EFG

3511. C₁₅H₂₁NO₂S₂2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-dithiolane**RN:** 35801-67-3**MP (°C):****MW:** 311.47**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	7.787E-03	rt	B174	0 0 1 0 1	

3512. C₁₅H₂₁NO₃Acetamide, 2-(benzoyloxy)-*N,N*-bis(1-methylethyl)-**RN:** 106231-56-5**MP (°C):** 105.5**MW:** 263.34**BP (°C):** 391.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.557E-04	1.200E-01	22	B427	1 0 0 1 1	in 0.01M HCl
4.557E-04	1.200E-01	22	N317	1 1 2 1 2	

3513. C₁₅H₂₁NO₃Acetamide, 2-(benzoyloxy)-*N*-hexyl-**RN:** 115193-29-8**MP (°C):** 130.5**MW:** 263.34**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-04	3.300E-02	22	N317	1 1 2 1 2	

3514. C₁₅H₂₁NO₃Acetamide, 2-(benzoyloxy)-*N,N*-dipropyl-**RN:** 106231-55-4**MP (°C):** 20**MW:** 263.34**BP (°C):** 402.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.177E-03	1.100E+00	22	B427	1 0 0 1 1	in 0.01M HCl
4.177E-03	1.100E+00	22	N317	1 1 2 1 2	

3515. C₁₅H₂₁NO₃S2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-oxathiolane

RN: 24606-94-8 MP (°C):

MW: 295.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.772E-02	rt	B174	0 0 1 0 0	

3516. C₁₅H₂₁NO₄

Metalaxyll

Methyl *N*-(2,6-dimethyl-phenyl)-*N*-(2'-methoxyacetyl)-DL-alaninate

Apron

Ridomil

Subdue

Fubol

RN: 57837-19-1 MP (°C): 72

MW: 279.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.488E-02	6.951E+00	20	E048	1 2 1 1 2	

3517. C₁₅H₂₁NO₄

Hexyl acetaminophen

Carbonic acid, 4-(acetylaminophenyl)hexyl ester

Acetanilide, 4'-hydroxy-, hexyl carbonate (ester)

RN: 17239-22-4 MP (°C): 112.5-113.5

MW: 279.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.325E-04	3.700E-02	37	D029	0 0 0 0 0	

3518. C₁₅H₂₁NO₄2-(*p*-Isopropylphenyl)-2-methyl-4-(methoxycarbamyl)-1,3-dioxolane

RN: 35858-24-3 MP (°C):

MW: 279.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.514E-01	rt	B174	0 0 1 0 0	

3519. C₁₅H₂₁NO₅Acetamide, 2-(benzoyloxy)-*N,N*-bis(2-methoxyethyl)-

RN: 115178-64-8 MP (°C): 57.5

MW: 295.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.672E-02	7.890E+00	22	N317	1 1 2 1 2	

3520. C₁₅H₂₁NO₅

Acetamide, 2-(benzoyloxy)-N,N-bis(2-hydroxypropyl)-

RN: 115178-63-7 MP (°C): 105.5

MW: 295.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.636E-02	1.960E+01	22	N317	1 1 2 1 2	

3521. C₁₅H₂₁N₂O₃

C.I. Disperse red 11

RN: 2872-48-2 MP (°C): 242

MW: 277.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-06	6.934E-04	25	B333	0 0 0 0 0	

3522. C₁₅H₂₁N₃O

Primaquine

Primaquine phosphate

Neo-quipenyl

8-(4-Amino-1-methylbutylamino)-6-methoxyquinoline

8-((4-Amino-1-methylbutyl)amino)-6-methoxyquinoline phosphate

Palum

RN: 90-34-6 MP (°C):

MW: 259.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.770E+00	7.184E+02	25	B443	0 0 0 0 0	

3523. C₁₅H₂₁N₅O₅

9-(2-O-Valeryl-β-D-arabinofuranosyl)adenine

RN: 87984-85-8 MP (°C):

MW: 351.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.960E-04	1.040E-01	37	B306	1 2 0 1 2	pH 7.3

3524. C₁₅H₂₁N₅O₅

9-[5'-(O-Isovaleryl)-β-D-arabinofuranosyl]adenine ester

RN: 65926-32-1 MP (°C):

MW: 351.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.635E-02	1.980E+01	ns	B134	0 1 1 1 2	

3525. C₁₅H₂₁N₅O₅

9-[5'-(O-Valeryl)-β-D-arabinofuranosyl]adenine ester

RN: 65926-31-0 MP (°C):

MW: 351.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.391E-02	8.400E+00	ns	B134	0 1 1 1 1	

3526. C₁₅H₂₁N₅O₅

9-[5'-(O-Pivaloyl)-β-D-arabinofuranosyl]adenine ester

RN: 65926-33-2 MP (°C):

MW: 351.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.992E-02	7.000E+00	ns	B134	0 1 1 1 1	

3527. C₁₅H₂₁N₅O₆

9-(1,3-Dipropionate-2-propoxymethyl)guanine

RN: 86357-20-2 MP (°C): 192

MW: 367.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.622E-03	2.800E+00	25	B360	0 0 0 0 0	

3528. C₁₅H₂₂ClNO₂

Metolachlor

2-Chloro-N-(2-ethyl-6-methylphenyl)-N-(2-methoxy-1-methylethyl)acetamide

Dual

Cotoran Multi

Ontrack 8E

Bicep 6L

RN: 51218-45-2 MP (°C): <25

MW: 283.80 BP (°C): 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.867E-03	5.297E-01	20	E048	1 2 1 1 2	
1.868E-03	5.300E-01	20	M161	1 0 0 0 2	
1.866E-03	5.297E-01	ns	S460	0 0 0 0 0	
1.868E-03	5.300E-01	ns	V414	0 0 0 0 0	

3529. C₁₅H₂₂ClNO₂

CP 52223

2-Chloro-N-(2,6-dimethyl)phenyl-N-isopropoxymethylacetamide

RN: 24353-58-0 MP (°C):

MW: 283.80 BP (°C): 137.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.079E-04	5.900E-02	ns	M061	0 0 0 0 1	

3530. C₁₅H₂₂N₂O

DL-Mepivacaine

Carbocaine

1-Methyl-2',6'-pipecoloxylidide

Carbocain

RN: 96-88-8 MP (°C): 150

MW: 246.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-02	3.350E+00	14.9	N046	2 0 1 1 1	intrinsic
3.653E-02	9.000E+00	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
2.841E-02	7.000E+00	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
9.000E-03	2.217E+00	25	D402	1 2 2 2 0	EFG
1.020E-02	2.513E+00	25	N046	2 0 1 1 1	intrinsic
9.910E-03	2.441E+00	34.5	N046	2 0 1 1 1	intrinsic
1.000E-02	2.464E+00	37	D402	1 2 2 2 0	EFG
7.970E-03	1.963E+00	37	N044	2 1 1 2 2	intrinsic

3531. C₁₅H₂₂O₃

Gemfibrozil

2,2-Dimethyl-5-(2,5-xylyloxy)valeric acid

Jezil

Lobid

Lopid

RN: 25812-30-0 MP (°C):

MW: 250.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.00E-03	>5.00E-01	ns	B404	0 2 1 1 0	

3532. C₁₅H₂₂O₃Octyl *p*-hydroxybenzoate*n*-Octyl 4-hydroxybenzoate

RN: 1219-38-1 **MP (°C):** 54
MW: 250.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.470E-05	3.680E-03	15	B355	0 0 0 0 0	
2.300E-04	5.758E-02	20	B355	0 0 0 0 0	
4.650E-04	1.164E-01	25	B355	0 0 0 0 0	
3.273E-03	8.193E-01	25	D081	1 2 2 1 2	
3.162E-04	7.916E-02	25	F322	2 0 1 1 0	EFG

3533. C₁₅H₂₂O₅

Octyl gallate

Octyl 3,4,5-trihydroxybenzoate

n-Octyl gallate

RN: 1034-01-1 **MP (°C):**
MW: 282.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.084E-05	2.000E-02	29.99	L430	0 0 0 0 0	
8.500E-05	2.400E-02	34.99	L430	0 0 0 0 0	
1.133E-04	3.200E-02	39.99	L430	0 0 0 0 0	
1.806E-04	5.100E-02	44.99	L430	0 0 0 0 0	
3.152E-04	8.899E-02	49.99	L430	0 0 0 0 0	
4.214E-04	1.190E-01	54.99	L430	0 0 0 0 0	
4.710E-04	1.330E-01	59.99	L430	0 0 0 0 0	
5.064E-04	1.430E-01	64.99	L430	0 0 0 0 0	

3534. C₁₅H₂₃NO₂Octyl *m*-aminobenzoate

Octyl 3-aminobenzoate

RN: 52222-35-2 **MP (°C):**
MW: 249.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	7.481E-03	ns	M066	0 0 0 0 0	

3535. C₁₅H₂₃NO₂Octyl *p*-aminobenzoate

4-Aminobenzoic acid octyl ester

RN: 14309-41-2 **MP (°C):**
MW: 249.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-06	7.979E-04	37	F006	1 1 2 2 1	

3536. C₁₅H₂₃NO₂

Alprenolol

Aptin

RN: 13655-52-2 **MP (°C):**
MW: 249.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.471E-03	3.669E-01	22.5	B422	0 0 0 0 0	

3537. C₁₅H₂₃NO₃

Parethoxycaine

4-Ethoxybenzoic acid-2-(diethylamino)ethyl ester

RN: 94-23-5 **MP (°C):** 173.0
MW: 265.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.930E-03	5.121E-01	ns	M066	0 0 0 0 2	

3538. C₁₅H₂₃NO₄

Cycloheximide

3-((R)-2-((1S,3S,5S)-3,5-Dimethyl-2-oxocyclohexyl)-2-hydroxyethyl)glutarimide

Actidione

Actispray

Naramycin

Kaken

RN: 66-81-9 **MP (°C):** 116.3
MW: 281.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.464E-02	2.100E+01	2	M161	1 0 0 0 1	

3539. C₁₅H₂₃N₃O₄

Isopropalin

2,6-Dinitro-N,N-dipropylcumidene

4-Isopropyl-2,6-dinitro-N,N-dipropylaniline

2,6-Dinitro-N,N-dipropylcumidine

Paarlan

Paarlan EC

RN: 33820-53-0 **MP (°C):**
MW: 309.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.232E-07	1.000E-04	25	M161	1 0 0 0 0	

3540. C₁₅H₂₃N₃O₄S

Sulpiride

N-[(1-Ethyl-2-pyrrolidinyl)methyl]-2-methoxy-5-sulfamoylbenzamide

RN: 15676-16-1 MP (°C):

MW: 341.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.15E-04	<2.10E-01	25	P312	0 0 0 0 0	

3541. C₁₅H₂₃N₃O₄S

Cyclacillin

Anhydrous 6-(1-aminocyclohexanecarboxamido)penicillanic acid

RN: 3485-14-1 MP (°C):

MW: 341.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.611E-01	5.500E+01	7	P035	0 0 0 0 0	EFG
1.054E-01	3.600E+01	20	P035	0 0 0 0 0	EFG
9.372E-02	3.200E+01	25	P035	0 0 0 0 0	EFG
7.908E-02	2.700E+01	30	P035	0 0 0 0 0	EFG
6.736E-02	2.300E+01	40	P035	0 0 0 0 0	EFG
6.151E-02	2.100E+01	50	P035	0 0 0 0 0	EFG
5.858E-02	2.000E+01	60	P035	0 0 0 0 0	EFG

3542. C₁₅H₂₃N₃O₄S·2H₂O

Cyclacillin (dihydrate)

Dihydrate 6-(1-aminocyclohexanecarboxamido)penicillanic acid

RN: 3485-14-1 MP (°C):

MW: 377.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.709E-02	1.400E+01	10	P035	0 0 0 0 0	EFG
3.709E-02	1.400E+01	20	P035	0 0 0 0 0	EFG
3.656E-02	1.380E+01	25	P035	0 0 0 0 0	EFG
3.656E-02	1.380E+01	30	P035	0 0 0 0 0	EFG
3.682E-02	1.390E+01	40	P035	0 0 0 0 0	EFG
3.762E-02	1.420E+01	50	P035	0 0 0 0 0	EFG
4.504E-02	1.700E+01	60	P035	0 0 0 0 0	EFG

3543. C₁₅H₂₄NO₄PS

Isofenphos

Methylethyl 2-((ethoxy((1-methylethyl)amino)phosphinothioyl)oxy)benzoate

Amaze

Oftanol

Pryfon

RN: 25311-71-1 **MP (°C):**
MW: 345.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.399E-05	2.210E-02	20	B300	2 1 1 1 2	<i>sic</i>
6.891E-02	2.380E+01	20	M161	1 0 0 0 2	<i>sic</i>

3544. C₁₅H₂₄N₂O₂N,N,N'-Triethyl-bicyclo(2.2.1)hept-5-ene-2,3-*trans*-dicarboxamide

RN: 62249-37-0 **MP (°C):**
MW: 264.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.232E-01	5.900E+01	20	K050	1 1 1 1 2	

3545. C₁₅H₂₄N₂O₂

Tetracaine

Pantocaine

Cetacaine

RN: 94-24-6 **MP (°C):**
MW: 264.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-04	1.560E-01	ns	E031	0 0 2 1 2	

3546. C₁₅H₂₄N₂O₂

4-Ethylaminobenzoic acid-2-(diethyl-amino)ethyl ester

RN: 16488-53-2 **MP (°C):**
MW: 264.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.600E-03	1.216E+00	ns	M066	0 0 0 0 1	

3547. C₁₅H₂₄N₂O₂

4-Aminobenzoic acid-2-(diethyl-amino)butyl ester
 2-(Diethyl(amino)butyl 4-aminobenzoate

RN: 5878-14-8 **MP (°C):**
MW: 264.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	1.137E+00	ns	M066	0 0 0 0 1	

3548. C₁₅H₂₄N₂O₃

2,4-Diazaspiro[5.11]heptadecane-1,3,5-trione

RN: 143288-64-6 **MP (°C):**
MW: 280.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-06	4.486E-04	25	P350	0 0 0 0 0	intrinsic

3549. C₁₅H₂₄O

Butylated hydroxytoluene
 2,6-Di-*tert*-butyl-*p*-cresol
 2,6-Di-*tert*-butyl-1-hydroxy-4-methylbenzene
 4-Hydroxy-3,5-di-*tert*-butyltoluene

RN: 128-37-0 **MP (°C):** 71
MW: 220.36 **BP (°C):** 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.54E-05	<1.00E-02	25	P312	0 0 0 0 0	

3550. C₁₅H₂₄O

4-Nonylphenol
 4-*t*-Nonylphenol

RN: 104-40-5 **MP (°C):**
MW: 220.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.090E-05	4.605E-03	2	A335	0 0 0 0 0	
2.088E-05	4.600E-03	2	A335	0 0 0 0 0	
2.230E-05	4.914E-03	10	A335	0 0 0 0 0	
2.233E-05	4.920E-03	10	A335	0 0 0 0 0	
2.380E-05	5.245E-03	14	A335	0 0 0 0 0	
2.378E-05	5.240E-03	14	A335	0 0 0 0 0	
2.470E-05	5.443E-03	20.5	A335	0 0 0 0 0	
2.464E-05	5.430E-03	20.5	A335	0 0 0 0 0	
2.882E-05	6.350E-03	25	A335	0 0 0 0 0	
2.890E-05	6.368E-03	25	A335	0 0 0 0 0	
3.177E-05	7.000E-03	25	M127	1 0 0 0 0	

3551. C₁₅H₂₄O

Nonylphenol

RN: 25154523

MP (°C):

MW: 220.36

BP (°C): 293–297

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.224E-05	4.900E-03	25	B420	1 1 1 1 1	

3552. C₁₅H₂₆N₂

Sparteine

(-)-Spartein

RN: 90-39-1

MP (°C): 30

MW: 234.39

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.297E-02	3.040E+00	22	F300	1 0 0 0 2	
1.297E-02	3.040E+00	25	D004	0 0 0 0 0	

3553. C₁₅H₂₆N₂O₃

5-Allyl-5-methylhexylcarbinylbarbituric acid

RN: MP (°C):

MW: 282.39

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.084E-02	3.060E+00	ns	T003	0 0 0 0 2	

3554. C₁₅H₂₆N₂O₃5-Ethyl-5-*n*-nonylbarbituric acid

5-Ethyl-5-nonylbarbiturate

RN: 64810-91-9 MP (°C):

MW: 282.39

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.450E-04	9.742E-02	25	M310	2 2 2 2 2	

3555. C₁₅H₂₆O₆

Tributyrin

Glyceryl tributyrate

Tributanoylglycerol

1,2,3-Propanetriyl tributyrate

RN: 60-01-5 MP (°C): 173

MW: 302.37 BP (°C): 287.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.307E-04	9.999E-02	ns	F014	0 0 0 0 1	

3556. C₁₅H₂₈O₄

1,13-Tridecanedicarboxylic acid

1,15-Pentadecanoic acid

RN: 1460-18-0 **MP (°C):**
MW: 272.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.285E-03	3.500E-01	21	B040	1 0 1 1 1	<i>sic</i>

3557. C₁₅H₃₀

1-Pentadecene

RN: 13360-61-7 **MP (°C):**
MW: 210.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.778E-09	3.740E-07	23	C332	0 0 0 0 0	

3558. C₁₅H₃₀O₂

Pentadecylic acid

Pentadecanoic acid

RN: 1002-84-2 **MP (°C):** 52
MW: 242.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.135E-05	7.600E-03	0	B136	1 0 2 1 1	
4.950E-05	1.200E-02	20	B136	1 0 2 1 1	
4.950E-05	1.200E-02	20.0	R001	1 1 1 1 1	
5.775E-05	1.400E-02	30	B136	1 0 2 1 1	
5.775E-05	1.400E-02	30.0	R001	1 1 1 1 1	
7.013E-05	1.700E-02	45	B136	1 0 2 1 1	
7.013E-05	1.700E-02	45.0	R001	1 1 1 1 1	
8.251E-05	2.000E-02	60	B136	1 0 2 1 1	
8.250E-05	2.000E-02	60.0	R001	1 1 1 1 1	
3.135E-05	7.600E-03	.0	R001	1 1 1 1 1	

3559. C₁₅H₃₀O₃

Dodecyl lactate

Propanoic acid, 2-hydroxy-, dodecyl ester

RN: 6283-92-7 **MP (°C):**
MW: 258.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.870E-04	1.000E-01	25	R006	2 2 0 1 0	

3560. C₁₅H₃₂

Pentadecane

n-Pentadecane

Pentadecane-d32

Pentadecane (*n*)

RN: 629-62-9

MP (°C): 9.9

MW: 212.42

BP (°C): 270.63

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.883E-10	4.000E-08	25	T423	0 0 0 0 0	

3561. C₁₅H₃₂O

Pentadecanol

Pentadecan-1-ol

1-Pentadecanol

RN: 629-76-5

MP (°C): 46

MW: 228.42

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-07	1.028E-04	25	R002	0 0 0 0 0	

3562. C₁₆H₈Cl₂F₆N₂O₃

Hexaflumuron

RN: 86479-06-3

MP (°C):

MW: 461.15

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.513E-08	1.620E-05	20	M402	0 0 0 0 0	

3563. C₁₆H₁₀

Fluoranthene

1,2-Benzacenaphthene

1,2-(1,8-Naphthalenediyl)benzene

Benzo[j,k]fluorene

Idryl

FA

RN: 206-44-0

MP (°C): 107

MW: 202.26

BP (°C): 384

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.050E-07	8.191E-05	8.10	M082	1 1 1 2 2	
4.050E-07	8.191E-05	8.10	M151	2 1 2 2 2	
4.058E-07	8.207E-05	8.14	M183	1 1 1 1 2	
5.290E-07	1.070E-04	13.20	M082	1 1 1 2 2	
5.290E-07	1.070E-04	13.20	M151	2 1 2 2 2	

(continued)

3563. C₁₆H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.295E-07	1.071E-04	13.24	M183	1 1 1 1 2	
7.330E-07	1.483E-04	19.70	M082	1 1 1 2 2	
7.330E-07	1.483E-04	19.70	M151	2 1 2 2 2	
7.339E-07	1.484E-04	19.74	M183	1 2 1 1 2	
1.190E-06	2.407E-04	20	E009	1 0 0 1 2	
9.394E-07	1.900E-04	20	H300	1 1 2 2 1	
8.850E-07	1.790E-04	20	V416	0 0 0 0 0	
5.933E-07	1.200E-04	24	H116	2 1 0 0 2	
1.000E-06	2.023E-04	24.60	M082	1 1 1 2 2	
1.000E-06	2.023E-04	24.60	M151	2 1 2 2 2	
1.003E-06	2.028E-04	24.64	M183	1 2 1 1 2	
1.400E-06	2.832E-04	25	A325	2 1 2 2 1	
1.023E-06	2.070E-04	25	D406	1 2 2 2 2	
1.320E-06	2.670E-04	25	K001	2 2 2 2 2	
1.335E-06	2.700E-04	25	L332	1 1 1 1 2	
1.285E-06	2.600E-04	25	M064	1 1 2 2 1	
1.019E-06	2.060E-04	25	M071	2 2 2 2 2	
1.300E-06	2.629E-04	25	M342	1 0 1 1 1	
1.167E-06	2.360E-04	25	S227	1 2 1 1 2	
1.019E-06	2.060E-04	25.00	M151	2 1 1 2 2	
1.187E-06	2.400E-04	27	D003	1 0 0 1 1	
1.305E-06	2.640E-04	29	M071	2 2 2 2 2	
1.305E-06	2.640E-04	29.00	M151	2 1 1 2 2	
1.380E-06	2.791E-04	29.90	M082	1 1 1 2 2	
1.380E-06	2.791E-04	29.90	M151	2 1 2 2 2	
1.382E-06	2.796E-04	29.94	M183	1 2 1 1 2	
2.947E-06	5.960E-04	40	V416	0 0 0 0 0	
8.464E-06	1.712E-03	60	V416	0 0 0 0 0	
1.300E-06	2.630E-04	ns	I332	0 0 0 0 1	

3564. C₁₆H₁₀

Pyrene

Benzo[def]phenanthrene

RN: 129-00-0 MP (°C): 156
 MW: 202.26 BP (°C): 404

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-07	<2.02E-05	4	K049	1 2 1 1 0	
2.430E-07	4.915E-05	4.70	M082	1 1 1 2 2	
2.430E-07	4.915E-05	4.70	M151	2 1 2 2 2	
2.434E-07	4.924E-05	4.74	M183	1 2 1 1 2	
2.890E-07	5.845E-05	9.50	M082	1 1 1 2 2	
2.890E-07	5.845E-05	9.50	M151	2 1 2 2 2	
2.895E-07	5.855E-05	9.54	M183	1 2 1 1 2	
3.560E-07	7.200E-05	14.30	M082	1 1 1 2 2	
3.560E-07	7.200E-05	14.30	M151	2 1 2 2 2	
3.563E-07	7.206E-05	14.34	M183	1 2 1 1 2	

(continued)

3564. C₁₆H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.588E-07	7.258E-05	15	B385	0 0 0 0 0	
4.610E-07	9.324E-05	18.70	M082	1 1 1 2 2	
4.610E-07	9.324E-05	18.70	M151	2 1 2 2 2	
4.617E-07	9.338E-05	18.74	M183	1 2 1 1 2	
5.200E-07	1.052E-04	20	E009	1 0 0 0 1	
5.200E-07	1.052E-04	20	E025	1 0 1 2 1	
4.700E-07	9.506E-05	20	H306	1 0 1 2 1	
5.370E-07	1.086E-04	21.20	M082	1 1 1 2 2	
5.370E-07	1.086E-04	21.20	M151	2 1 2 2 2	
5.394E-07	1.091E-04	21.24	M183	1 2 1 1 2	
7.200E-07	1.456E-04	22	A413	2 0 2 2 1	
6.279E-07	1.270E-04	22.20	W003	2 1 2 2 2	average of 3
6.675E-07	1.350E-04	24	H106	1 0 2 2 2	
1.582E-07	3.200E-05	24	H116	2 1 0 0 1	
6.675E-07	1.350E-04	24	M129	1 2 1 1 2	
5.834E-07	1.180E-04	25	B319	2 0 1 2 2	
6.490E-07	1.313E-04	25	B385	0 0 0 0 0	
7.700E-07	1.557E-04	25	K001	1 0 2 1 2	
4.700E-07	9.506E-05	25	K123	1 0 2 2 1	
7.911E-07	1.600E-04	25	L332	1 1 1 1 2	
6.675E-07	1.350E-04	25	M064	1 1 2 2 2	
6.526E-07	1.320E-04	25	M071	2 2 2 2 2	
6.675E-07	1.350E-04	25	M156	1 2 1 1 2	
6.670E-07	1.349E-04	25	M342	1 0 1 1 2	
3.955E-07	8.000E-05	25	P340	0 0 0 0 0	
3.556E-08	7.191E-06	25	R084	2 2 2 2 1	sic
7.400E-07	1.497E-04	25	R302	1 2 1 2 1	
8.455E-07	1.710E-04	25	S227	1 2 1 1 2	
6.526E-07	1.320E-04	25.00	M151	2 1 1 2 2	
6.730E-07	1.361E-04	25.50	M082	1 1 1 2 2	
6.730E-07	1.361E-04	25.50	M151	2 1 2 2 2	
6.728E-07	1.361E-04	25.54	M183	1 2 1 1 2	
8.158E-07	1.650E-04	27	D003	1 0 0 1 1	
8.010E-07	1.620E-04	29	M071	2 2 2 2 2	
8.010E-07	1.620E-04	29.00	M151	2 1 1 2 2	
8.390E-07	1.697E-04	29.90	M082	1 1 1 2 2	
8.390E-07	1.697E-04	29.90	M151	2 1 2 2 2	
8.411E-07	1.701E-04	29.94	M183	1 2 1 1 2	
1.147E-06	2.320E-04	34.50	W003	2 1 2 2 2	average of 2
9.888E-07	2.000E-04	35	B385	0 0 0 0 0	
1.973E-06	3.990E-04	44.70	W003	2 1 2 2 2	average of 3
2.784E-06	5.630E-04	50.10	W003	2 1 2 2 2	average of 3
3.758E-06	7.600E-04	55.60	W003	2 1 2 2 1	average of 3
3.659E-06	7.400E-04	56.00	W003	2 1 2 2 1	
4.648E-06	9.400E-04	60.70	W003	2 1 2 2 1	average of 3
6.329E-06	1.280E-03	65.20	W003	2 1 2 2 2	average of 2
9.196E-06	1.860E-03	71.90	W003	2 1 2 2 2	average of 3
1.093E-05	2.210E-03	74.70	W003	2 1 2 2 2	
6.675E-07	1.350E-04	ns	H123	0 0 0 0 0	

(continued)

3564. C₁₆H₁₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.675E-07	1.350E-04	ns	K304	0 0 0 0 2	
6.675E-07	1.350E-04	ns	M344	0 0 0 0 2	
5.000E-07	1.011E-04	ns	M383	0 2 1 1 0	
1.000E-06	2.023E-04	ns	W005	0 0 1 2 0	

3565. C₁₆H₁₀N₂O₈S₂

C.I. Acid blue 74(free acid)

Indigo-disulfosaeure-(5,5')

Indigotinsulfonic acid

RN: 860-22-0 MP (°C):

MW: 422.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~2.37E-02	~1.00E+01	25	F300	1 0 0 0 0	

3566. C₁₆H₁₁NO₂

Cinchophen

2-Phenyl-4-quinolinecarboxylic acid

2-Phenylcinchoninic acid

RN: 132-60-5 MP (°C): 213

MW: 249.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.418E-04	1.600E-01	25	L074	2 2 1 1 2	

3567. C₁₆H₁₂F₃NO

6H-Dibenz[b,e]azepin-6-one, 5,11-dihydro-5-(2,2,2-trifluoroethyl)-

RN: 155206-49-8 MP (°C):

MW: 291.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.589E-05	4.627E-03	ns	M381	0 1 1 1 2	pH 7.0

3568. C₁₆H₁₂N₂O₃

5,5-Diphenylbarbituric acid

2,4,6(1H,3H,5H)-Pyrimidinetrione, 5,5-diphenyl

Barbituric acid, 5,5-diphenyl

5,5-Diphenylbarbiturate

RN: 21914-07-8 MP (°C):

MW: 280.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.370E-05	1.785E-02	25	P350	0 0 0 0 0	intrinsic

3569. C₁₆H₁₂N₂O₄S

Sulfanaphthoquinone

RN:

MW: 328.35

MP (°C):

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	4.500E-02	20	F073	1 2 2 2 1	

3570. C₁₆H₁₂O₆

Hematein

Haematein

Benz[b]indeno[1,2-d]pyran-9(6H)-one, 6α,7-dihydro-3,4,6α,10-tetrahydroxy-

RN: 475-25-2 MP (°C): >200

MW: 300.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.998E-03	6.000E-01	20	F300	1 0 0 0 1	

3571. C₁₆H₁₂O₆

Benzoic acid, 2-(acetyloxy)-, 2-carboxyphenyl ester

RN: 530-75-6 MP (°C): 166.5

MW: 300.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.661E-05	2.000E-02	21	N335	0 0 0 0 0	

3572. C₁₆H₁₃ClN₂O

Diazepam

7-Chloro-1-methyl-5-phenyl-2H-1,4-benzodiazepin-2-one

Valium

Valrelease

Vazepam

Diazemuls

RN: 439-14-5 MP (°C): 125

MW: 284.75 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.475E-04	4.200E-02	20	N059	2 0 2 2 2	average of 2
1.756E-04	5.000E-02	25	G084	2 0 2 2 1	
1.756E-04	5.000E-02	25	G095	2 1 2 2 1	
1.756E-04	5.000E-02	25	M159	1 0 2 2 0	EFG, pH 7.0
2.320E-04	6.606E-02	25	M320	2 2 1 1 2	
1.089E-04	3.100E-02	25	M457	0 0 0 0 0	
1.510E-04	4.300E-02	25	N055	2 0 2 2 1	
1.580E-04	4.500E-02	25	N055	2 0 2 1 2	

(continued)

3572. C₁₆H₁₃ClN₂O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.721E-04	4.900E-02	25	N055	2 0 2 1 2	
1.405E-04	4.000E-02	30	R081	1 2 2 2 0	
2.900E-04	8.258E-02	50	M335	1 0 2 1 2	pH 6.0
1.200E-04	3.417E-02	ns	F327	0 0 1 2 2	
3.512E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.756E-04	5.000E-02	ns	M036	0 0 0 0 0	

3573. C₁₆H₁₃Cl₂NO₄

Aceclofenac

RN: 89796-99-6 **MP (°C):**
MW: 354.19 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.034E-05	3.200E-02	32	C411	2 1 1 2 1	

3574. C₁₆H₁₃I₃N₂O₃

Iobenzamic acid

N-(3-Amino-2,4,6-triiodobenzoyl)-N-phenyl-β-alanine

Orbil

Osbiland

Razebil

Osbil

RN: 3115-05-7 **MP (°C):**
MW: 662.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.737E-04	1.150E-01	ns	H055	0 0 0 0 0	

3575. C₁₆H₁₃NO₃

C.I. Disperse red 3

N-(2-Hydroxyethyl)-1-aminoanthraquinone

Disperse red 3

Disperse red 66

RN: 4465-58-1 **MP (°C):** 168
MW: 267.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	4.277E-03	25	B333	0 0 0 0 0	

3576. C₁₆H₁₃N₃

Yellow AB

1-Phenylazo-2-naphthylamine

RN: 85-84-7 **MP (°C):** 102
MW: 247.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.213E-06	3.000E-04	37	H120	1 1 1 1 0	normal saline

3577. C₁₆H₁₃N₃O₃

Mebendazole

Methyl 5-benzoyl benzimidazole-2-carbamate

Pantelmin

Methyl 5-benzoyl-2-benzimidazolecarbamate

RN: 31431-39-7 **MP (°C):** 288.5
MW: 295.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.693E-06	5.000E-04	21	N337	0 0 0 0 0	pH 5
1.700E-06	5.020E-04	21	N337	0 0 0 0 0	pH 5
1.199E-04	3.540E-02	25	H075	1 0 2 1 2	polymorph C
2.414E-04	7.130E-02	25	H075	1 0 2 1 2	polymorph B
3.332E-05	9.840E-03	25	H075	1 0 2 1 2	polymorph A
3.725E-06	1.100E-03	288.5	D426	0 0 0 0 0	
1.318E-04	3.893E-02	ns	R427	0 0 0 0 0	

3578. C₁₆H₁₄

9,10-Dimethylanthracene

RN: 781-43-1 **MP (°C):** 182
MW: 206.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.715E-07	5.600E-05	25	M064	1 1 2 2 1	
2.700E-07	5.570E-05	25	M342	1 0 1 1 1	
2.715E-07	5.600E-05	ns	M344	0 0 0 0 2	

3579. C₁₆H₁₄ClN₃O

Chlordiazepoxide

7-Chloro-2-(methylamino)-5-phenyl-3H-1,4-benzodiazepine-4-oxide

Librium

Menrium

Tropium

SK-Lygen

RN: 58-25-3 MP (°C): 236

MW: 299.76 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.607E-03	1.981E+00	ns	R427	0 0 0 0 0	
6.672E-03	2.000E+00	rt	M035	0 0 0 0 0	

3580. C₁₆H₁₄Cl₂N₂O₂

Phenobenzuron

Benzoyl-1-(3,4-dichlorophenyl)-3,3-dimethylurea

Benzomarc

Urea, N-benzoyl-N-(3,4-dichlorophenyl)-N',N'-dimethyl-

RN: 3134-12-1 MP (°C): 119

MW: 337.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.745E-05	1.600E-02	22	M161	1 0 0 0 1	

3581. C₁₆H₁₄Cl₂O₃

Chlorobenzilate

Ethyl 4,4'-dichlorobenzilate

Acaraben

Benzilen

Folbex

Kopmite

RN: 510-15-6 MP (°C): 36

MW: 325.19 BP (°C): 157

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.998E-05	1.300E-02	20	F311	1 2 2 2 1	

3582. C₁₆H₁₄Cl₂O₄

Diclotop-methyl

Methyl (+/-)-2-[4-(2,4-dichlorophenoxy)phenoxy]propionate

RN: 51338-27-3 MP (°C): 40

MW: 341.19 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.465E-04	5.000E-02	22	M161	1 0 0 0 1	

3583. C₁₆H₁₄FNO

6H-Dibenz[b,e]azepin-6-one, 5-(2-fluoroethyl)-5,11-dihydro-

RN: 155206-48-7 **MP (°C):****MW:** 255.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.917E-04	7.448E-02	ns	M381	0 1 1 1 2	pH 7.0

3584. C₁₆H₁₄N₂O

Methaqualone

Quaalude

Mandrax

Somnafac

RN: 72-44-6 **MP (°C):** 114–117**MW:** 250.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.198E-03	2.999E-01	23	P094	0 0 0 0 0	

3585. C₁₆H₁₄N₂O₂

C.I. Disperse blue 14

9,10-Anthracenedione, 1,4-bis(methylamino)-

RN: 2475-44-7 **MP (°C):** 226**MW:** 266.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-07	3.728E-05	25	B333	0 0 0 0 0	

3586. C₁₆H₁₄N₂O₃

3-(Hydroxymethyl)phenytoin

3-(Hydroxymethyl)-5,5-diphenyl-2,4-imidazolidinedione

RN: 21616-46-6 **MP (°C):****MW:** 282.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.959E-04	1.400E-01	22	B154	1 1 1 1 1	0.1M HCl

3587. C₁₆H₁₄N₂O₄

C.I. Disperse blue 26

9,10-Anthracenedione, 1,5-dihydroxy-4,8-bis(methylamino)-

Resiren blue TG

Navilene blue GL

PTB 31

RN: 3860-63-7 MP (°C): 217

MW: 298.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.800E-08	2.028E-05	25	B333	0 0 0 0 0	

3588. C₁₆H₁₄O₃

Ketoprofen

2-(*meta*-Benzoylphenyl) propionic acid

Orudis

Alrheumat

Oruvail

RN: 22071-15-4 MP (°C): 94

MW: 254.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.509E-04	6.380E-02	5	F306	1 0 1 2 2	intrinsic
9.045E-04	2.300E-01	21	B331	1 2 2 1 1	pH 7.4
3.696E-04	9.399E-02	22.5	B422	2 0 2 2 2	
4.640E-04	1.180E-01	25	A408	2 0 1 2 0	int
2.006E-04	5.100E-02	25	A427	0 0 0 0 0	
5.646E-04	1.436E-01	25	F306	1 0 1 2 2	intrinsic
1.156E-03	2.939E-01	32	C411	2 1 1 2 1	
8.066E-04	2.051E-01	37	F306	1 0 1 2 2	intrinsic
5.112E-04	1.300E-01	37	Y421	0 0 0 0 0	
3.933E-05	1.000E-02	amb	L434	0 0 0 0 0	
2.006E-04	5.100E-02	rt	H302	0 0 2 1 2	intrinsic
8.219E-04	2.090E-01	rt	R431	0 0 0 0 0	Average

3589. C₁₆H₁₄O₃

Fenbufen

3-(4-Biphenylylcarbonyl) propionic acid

Lederfen

RN: 36330-85-5 MP (°C): 185

MW: 254.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-06	9.409E-04	5	F306	1 0 1 2 2	intrinsic
1.000E-05	2.543E-03	24.99	K447	0 0 0 0 0	pH 2.0
6.430E-05	1.635E-02	25	C314	0 0 0 0 0	
6.410E-05	1.630E-02	25	C314	0 0 0 0 0	
8.700E-06	2.212E-03	25	F301	1 1 0 0 1	pH 2.0, <i>sic</i> <i>(continued)</i>

3589. C₁₆H₁₄O₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-06	2.212E-03	25	F306	1 0 1 2 2	intrinsic
1.800E-05	4.577E-03	37	F306	1 0 1 2 2	intrinsic
7.865E-06	2.000E-03	rt	H302	0 0 2 1 1	intrinsic

3590. C₁₆H₁₅CIN₂

Medazepam

7-Chloro-2,3-dihydro-1-methyl-5-phenyl-1H-1,4-benzodiazepine

Nobrium

RN: 2898-12-6 MP (°C):

MW: 270.76 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.083E-02	37	L011	1 0 2 1 1	

3591. C₁₆H₁₅Cl₂NO₂

Clomeprop

2-(2,4-Dichloro-3-methylphenoxy)-N-phenylpropanamide

RN: 84496-56-0 MP (°C):

MW: 324.21 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-08	3.168E-05	ns	R427	0 0 0 0 0	

3592. C₁₆H₁₅Cl₃OS₂2-(*p*-Methylthiophenyl)-2-(*p*-methylsulfinylphenyl)-1,1,1-trichloroethane

RN: 28463-05-0 MP (°C): 133-136

MW: 393.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.174E-06	1.250E-03	ns	K117	0 1 2 1 1	

3593. C₁₆H₁₅Cl₃O₂

Methoxychlor

1,1'-(2,2,2-Trichloroethylidene)-bis[4-methoxybenzene]

Maralate

Methoxy DDT

Marlate

Chemform

RN: 72-43-5 MP (°C): 82.5

MW: 345.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.786E-08	2.000E-05	15	B083	2 2 1 2 1	particle size 5 µm
1.302E-07	4.500E-05	25	B083	2 2 1 2 1	particle size 5 µm

(continued)

3593. C₁₆H₁₅Cl₃O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.447E-07	5.000E-05	25	P085	0 0 0 0 0	
2.893E-07	1.000E-04	25	W025	1 0 2 2 2	
2.748E-07	9.500E-05	35	B083	2 2 1 2 1	particle size 5 µm
5.352E-07	1.850E-04	45	B083	2 2 1 2 2	particle size 5 µm
1.794E-06	6.200E-04	ns	K117	0 1 2 1 1	
8.679E-09	3.000E-06	ns	K138	0 0 0 0 2	
2.314E-06	8.000E-04	ns	M110	0 0 0 0 0	EFG
1.794E-06	6.200E-04	ns	M138	0 1 0 0 1	
3.472E-07	1.200E-04	ns	M344	0 0 0 0 1	
2.089E-07	7.222E-05	ns	R427	0 0 0 0 0	

3594. C₁₆H₁₅Cl₃O₂S₂2,2-bis(*p*-Methylsulfinylphenyl)-1,1,1-trichloroethane2-(*p*-Methylsulfoxidephenyl)-1,1,1-trichloroethane

RN: 28396-87-4 MP (°C): 150–153

MW: 409.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.077E-05	2.900E-02	ns	K117	0 1 2 1 1	

3595. C₁₆H₁₅Cl₃O₄S₂2,2-bis(*p*-Methylsulfonylphenyl)-1,1,1-trichloroethane

RN: 30665-94-2 MP (°C): 236.0

MW: 441.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.395E-06	1.500E-03	ns	K117	0 1 2 1 1	

3596. C₁₆H₁₅Cl₃S₂2,2-bis(*p*-Methylthiophenyl)-1,1,1-trichloroethane

RN: 19679-38-0 MP (°C): 115–117

MW: 377.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.509E-06	5.700E-04	ns	K117	0 1 2 1 1	

3597. C₁₆H₁₅FN₂O₅

1-Butyryloxymethyl-3-benzoyl-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

1-Butyryloxymethyl-3-benzoyl-5-fluorouracil

RN: 97108-48-0 MP (°C): 81–82

MW: 334.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.855E-04	6.200E-02	22	B321	0 0 0 0 0	pH 4.0

3598. C₁₆H₁₅NO

4-Cyano-4'-propyloxybiphenyl

3 COB

RN: 52709-86-1 **MP (°C):**
MW: 237.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-07	2.136E-04	21	D300	2 2 1 1 2	

3599. C₁₆H₁₅NO₂

N-Butyl-1,8-naphthalimide

Naphthalimide, *N*-butyl-

1H-Benz[de]isoquinoline-1,3(2H)-dione, 2-butyl-

RN: 6914-62-1 **MP (°C):** 95
MW: 253.30 **BP (°C):** 412.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	5.066E-03	23	B410	2 1 2 2 2	

3600. C₁₆H₁₅NO₂

Cinnamyl anthranilate

2-Propen-1-ol, 3-phenyl-, 2-aminobenzoate

2-Aminobenzoic acid 3-phenyl-2-propenyl ester

3-Phenyl-2-propen-1-yl anthranilate

3-Phenyl-2-propenyl 2-aminobenzoate

Cinnamyl alcohol

RN: 87-29-6 **MP (°C):** 60
MW: 253.30 **BP (°C):** 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.080E-07	2.300E-04	ns	B338	0 0 0 0 1	

3601. C₁₆H₁₅NO₃

Benzoylphenylalanine

N-Benzoyl-DL-phenylalanine

RN: 2901-76-0 **MP (°C):**
MW: 269.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.156E-03	8.500E-01	25.1	N026	0 0 0 0 0	

3602. C₁₆H₁₅NO₄

Benzoyltyrosine

N-Benzoyl-L-tyrosine

RN: 2566-23-6 **MP (°C):**
MW: 285.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.290E-02	3.680E+00	25.1	N026	0 0 0 0 0	

3603. C₁₆H₁₅N₅

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-nitrile, 11-cyclopropyl-5,11-dihydro-4-methyl

RN: **MP (°C):**
MW: 277.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.816E-05	5.035E-03	ns	M381	0 1 1 1 2	pH 7.0

3604. C₁₆H₁₅N₅O₄S

2,5-Disulfanilamidopyridine

RN: **MP (°C):**
MW: 373.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.326E-03	4.950E-01	37	R058	1 2 1 1 2	

3605. C₁₆H₁₆

1,2,3,6,7,8-Hexahydronaphthalene

RN: 1732-13-4 **MP (°C):** 133
MW: 208.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	2.291E-04	4	K049	1 0 2 1 1	

3606. C₁₆H₁₆ClN₃O₃S

Metolazone

2-Methyl-3-(*o*-tolyl)-6-sulfamyl-7-chloro-1,2,3,4-tetrahydro-4-quinazolinone

Zaroxolyn

Mykrox

Diulo

RN: 17560-51-9 **MP (°C):** 256.0
MW: 365.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.321E-05	3.410E-02	10	B030	1 0 1 1 2	
1.339E-04	4.900E-02	20	B030	1 0 1 1 2	

(continued)

3606. C₁₆H₁₆ClN₃O₃S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.648E-04	6.030E-02	25	B030	1 0 1 1 2	
1.971E-04	7.210E-02	30	B030	1 0 1 1 2	
2.236E-04	8.180E-02	35	B030	1 0 1 1 2	
2.733E-04	1.000E-01	36	B030	1 0 1 1 2	
1.640E-04	6.000E-02	37	H013	1 0 0 0 0	
2.952E-04	1.080E-01	40	B030	1 0 1 1 2	
3.799E-04	1.390E-01	45	B030	1 0 1 1 2	
4.155E-04	1.520E-01	50	B030	1 0 1 1 2	

3607. C₁₆H₁₆N₂

3,4,7,8-Tetramethyl-1,10-phenanthroline

RN: 1660-93-1 MP (°C): 278.5

MW: 236.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.400E-06	1.512E-03	25.04	B094	1 2 1 2 1	

3608. C₁₆H₁₆N₂O₄

Phenmedipham

Methyl *m*-hydroxycarbanilate *m*-methylcarbanilate

RN: 13684-63-4 MP (°C): 143

MW: 300.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.33E-05	<1.00E-02	20	B200	1 0 0 0 0	
3.330E-06	1.000E-03	20	F311	1 2 2 2 1	
1.397E-05	4.194E-03	25	H434	0 0 0 0 0	
3.330E-05	1.000E-02	ns	M061	0 0 0 0 1	
9.989E-06	3.000E-03	rt	M161	0 0 0 0 0	

3609. C₁₆H₁₆N₂O₄

Desmedipham

Ethyl *m*-hydroxycarbanilate carbanilateCarbamic acid, *N*-phenyl-, 3-((ethoxycarbonyl)amino)phenyl ester

Betanex

Betanal-475

Betamix 70 WP

RN: 13684-56-5 MP (°C): 120

MW: 300.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.331E-05	7.000E-03	rt	M161	0 0 0 0 0	
2.331E-05	7.000E-03	rt	R304	0 0 0 0 0	

3610. C₁₆H₁₆N₄

Disperse black 1

RN: 6054-48-4

MP (°C):

MW: 264.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-07	7.930E-05	25	B333	0 0 0 0 0	

3611. C₁₆H₁₆N₄O

6H-Dipyrido[3,2-b:2'3'-e][1,4]diazepin-6-one, 11-cyclopropyl-5,11-dihydro-2,4-dimethyl-

RN: 135794-77-3 MP (°C):

MW: 280.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.346E-05	1.499E-02	ns	M381	0 1 1 1 2	pH 7.0

3612. C₁₆H₁₆N₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-cyclobutyl-5,11-dihydro-5-methyl-

RN: 135794-88-6 MP (°C):

MW: 280.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.911E-04	8.160E-02	ns	M381	0 1 1 1 2	pH 7.0

3613. C₁₆H₁₆N₆O₄S

2,5-Disulfanilamidopyrimidine

RN: MP (°C):

MW: 388.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.664E-05	2.200E-02	37	R046	1 2 1 1 1	

3614. C₁₆H₁₆O₂

4-Methoxy-3,3'-dimethylbenzophenone

RN: 41295-28-7 MP (°C): 62.25

MW: 240.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.323E-06	2.000E-03	20	M161	1 0 0 0 0	

3615. C₁₆H₁₆O₃

Ethyl benzoyl benzoate

RN: 106396-19-4 **MP (°C):****MW:** 256.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.901E-04	9.999E-02	ns	F014	0 0 0 0 1	

3616. C₁₆H₁₆O₃

Anisyl phenylacetate

p-Methoxybenzyl phenylacetatePhenylacetic acid, *p*-methoxybenzyl ester**RN:** 102-17-0 **MP (°C):****MW:** 256.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	5.126E-01	25	D407	1 0 2 2 2	
2.000E-03	5.126E-01	ns	S460	0 0 0 0 0	

3617. C₁₆H₁₇CIN₂S

Chlorphenethazine

2-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-ethanamide**RN:** 2095-24-1 **MP (°C):****MW:** 304.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-05	4.573E-03	ns	G023	0 0 1 1 1	

3618. C₁₆H₁₇CIN₄O₃

C.I. Disperse red 13

4-Nitro-2-chloro-4'-[ethyl(2-hydroxyethyl)amino]azobenzene

Acetoquinone light rubine BLZ

Acetamine rubine B

Acetate fast rubine B

RN: 3180-81-2 **MP (°C):** 133**MW:** 348.79 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-08	1.151E-05	25	B333	0 0 0 0 0	

3619. C₁₆H₁₇CIN₄O₄

C.I. Disperse red 7

Ethanol, 2,2'-[[3-chloro-4-[(4-nitrophenyl)azo]phenyl]imino]bis-

RN: 4540-00-5 MP (°C): 190

MW: 364.79 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	4.013E-04	25	B333	0 0 0 0 0	

3620. C₁₆H₁₇NO

Diphenamid

Dyamid

Enide

N,N-Dimethyl- α -phenylbenzeneacetamide

N,N-Dimethyldiphenylacetamide

Diherbid

RN: 957-51-7 MP (°C): 132

MW: 239.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-03	2.399E-01	25	M061	1 0 0 0 1	
1.086E-03	2.600E-01	25	M161	1 0 0 0 2	
1.090E-03	2.609E-01	27	B200	1 0 0 0 2	
1.086E-03	2.600E-01	ns	B185	0 0 0 0 0	
2.079E-02	4.975E+00	ns	B200	0 0 0 0 0	
1.086E-03	2.600E-01	ns	H042	0 0 0 0 2	

3621. C₁₆H₁₇NO₄2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-amino-2-oxoethyl ester, (*S*)Naproxen, *N,N*-glycolamide ester2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-amino-2-oxoethyl esterNaproxen *N,N*-glycolamide ester

RN: 114665-17-7 MP (°C): 139.5

MW: 287.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.183E-04	3.400E-02	21	B331	1 2 2 1 2	pH 7.4
1.183E-04	3.400E-02	21	B331	0 0 0 0 0	

3622. C₁₆H₁₇N₃O₄S

Cephalexin

Cefanex

C-Lexin

Keflex

Cefalexin

RN: 15686-71-2 **MP (°C):**
MW: 347.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.724E-02	5.990E+00	10	O305	2 2 1 2 2	noncrystalline
1.569E-01	5.450E+01	15	O305	2 2 1 2 2	noncrystalline
1.416E-01	4.920E+01	20	O305	2 2 1 2 2	noncrystalline
3.598E-02	1.250E+01	25	P311	0 0 0 0 0	EFG
1.330E-02	4.620E+00	25	U001	0 0 0 0 0	
3.500E-03	1.216E+00	35	E311	0 0 0 0 0	

3623. C₁₆H₁₇N₃O₄S.H₂O

Cephalexin (monohydrate)

RN: 23325-78-2 **MP (°C):**
MW: 365.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.694E-02	1.350E+01	25	M165	1 0 0 0 2	

3624. C₁₆H₁₇N₅O₅

Dis. A. 12

Ethanol, 2-[[4-[(2,4-dinitrophenyl)azo]phenyl]ethylamino]-

RN: 62570-20-1 **MP (°C):**
MW: 359.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-06	7.187E-04	25	B333	0 0 0 0 0	

3625. C₁₆H₁₇N₅O₆

Dis. A. 14

4-[bis(2-Hydroxyethyl)amino]-2',4'-dinitroazobenzene

RN: 60129-67-1 **MP (°C):**
MW: 375.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-06	2.252E-03	25	B333	0 0 0 0 0	

3626. C₁₆H₁₈CINO₄S

Oxathiin carboxanilide

Benzoic acid, 2-chloro-5-[(5,6-dihydro-2-methyl-1,4-oxathiin-3-yl)carnonyl]amino]isopropyl Ester

RN: 135812-04-3 **MP (°C):** 130
MW: 355.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.653E-06	1.300E-03	25	O319	0 0 0 0 0	

3627. C₁₆H₁₈FN₃O₃

Norfloxacin

Noroxin

RN: 70458-96-7 **MP (°C):**
MW: 319.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.455E-04	2.700E-01	6	Y421	0 0 0 0 0	
6.576E-04	2.100E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
6.263E-04	2.000E-01	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer
2.505E-02	8.000E+00	25	A414	1 0 1 1 1	pH 5 citrate buffer (0.1 M)
5.950E-04	1.900E-01	25	A414	1 0 1 1 1	
1.159E-03	3.700E-01	25	Y421	0 0 0 0 0	
2.662E-03	8.500E-01	40	Y421	0 0 0 0 0	

3628. C₁₆H₁₈NO₅P

Diphenylmorpholidophosphate

RN: **MP (°C):**
MW: 335.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.844E-03	2.295E+00	25	A040	1 0 0 0 2	

3629. C₁₆H₁₈N₂O₃

Difenoxuron

N-4-(4'-Methoxyphenoxy)phenyl-N',N'-dimethylurea

C-3470

RN: 14214-32-5 **MP (°C):** 138.5
MW: 286.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.985E-05	2.000E-02	20	M161	1 0 0 0 1	
6.985E-05	2.000E-02	ns	M061	0 0 0 0 1	

3630. C₁₆H₁₈N₂O₄S

Penicillin G

Benzylpenicillin

Pfizerpen

RN: 61-33-6 **MP (°C):**
MW: 334.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	2.675E+00	25	U001	0 0 0 0 0	

3631. C₁₆H₁₈N₄O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-(1,1-dimethylethyl)-5,11-dihydro-5-methyl-

RN: 135794-80-8 **MP (°C):**
MW: 282.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.416E-05	3.997E-03	ns	M381	0 1 1 1 2	pH 7.0

3632. C₁₆H₁₈N₄O₂

Dye III

4{[(4-Diethylamino)phenyl]azo}nitrobenzene

RN: **MP (°C):**
MW: 298.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.100E-07	2.715E-04	97.40	B198	1 2 1 1 1	

3633. C₁₆H₁₈N₄O₂

Dis. A. 5

4-Nitro-4'-diethylaminoazobenzene

4-Nitro-4'-N,N-diethylaminoazobenzene

DEANAB

RN: 3025-52-3 **MP (°C):** 152
MW: 298.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-11	1.193E-08	25	B333	0 0 0 0 0	

3634. C₁₆H₁₈N₄O₃

Disperse red 1

Dye IV

C.I. Disperse red 1

1-[N-Ethyl-N-(2-hydroxyethyl)amino]-4-(4-nitrophenylazo)benzene

4-Nitro-4'-[ethyl(2-hydroxyethyl)amino]azobenzene

RN: 2872-52-8 **MP (°C):** 161**MW:** 314.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-07	1.697E-04	25	B333	0 0 0 0 0	
5.400E-06	1.697E-03	60	B198	1 2 1 1 1	
6.521E-06	2.050E-03	60	P313	0 0 0 0 0	average of 2
1.082E-05	3.400E-03	70	P313	0 0 0 0 0	average of 2
1.310E-05	4.118E-03	71.80	B198	1 2 1 1 2	
1.797E-05	5.650E-03	80	P313	0 0 0 0 0	average of 2
3.120E-05	9.808E-03	84.10	B198	1 2 1 1 2	
3.388E-05	1.065E-02	90	P313	0 0 0 0 0	average of 2
7.130E-05	2.241E-02	97.40	B198	1 2 1 1 2	

3635. C₁₆H₁₈N₄O₄

Disperse red 19

Dye V

C.I. Disperse red 19

2-[(2-Hydroxyethyl)[4-(4-nitrophenylazo)phenyl]amino]ethanol

4'-(*N,N*-Dihydroxyethyl)amino]-4-nitroazobenzene**RN:** 2734-52-3 **MP (°C):** 209**MW:** 330.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-07	2.345E-04	25	B333	0 0 0 0 0	
1.170E-05	3.865E-03	60	B198	1 2 1 1 2	
3.030E-05	1.001E-02	71.80	B198	1 2 1 1 2	
8.330E-05	2.752E-02	84.10	B198	1 2 1 1 2	
2.100E-04	6.937E-02	97.40	B198	1 2 1 1 2	

3636. C₁₆H₁₈O₃Naproxen ethyl ester^v2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, ethyl ester, (*alpha*S)-**RN:** 31220-35-6 **MP (°C):****MW:** 258.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.645E-06	1.200E-03	21	B331	1 2 2 1 2	pH 7.4
4.645E-06	1.200E-03	21	B331	0 0 0 0 0	

3637. C₁₆H₁₉ClN₂

Chlorpheniramine

1-(p-Chlorophenyl)-1-(2-pyridyl)-3-dimethylaminopropane

RN: 132-22-9 MP (°C): <25

MW: 274.80 BP (°C): 142

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-02	5.496E+00	37.5	L034	2 2 0 1 2	pH 7.4

3638. C₁₆H₁₉NO₇

Benzoic acid, 2-(acetoxy)-, 2-[(2-ethoxy-2-oxoethyl)methylamino]-2-oxoethyl ester

RN: 116482-77-0 MP (°C): 47.5

MW: 337.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.846E-03	9.600E-01	21	N335	0 0 0 0 0	

3639. C₁₆H₁₉N₃O₂

C.I. Solvent yellow 58

p-[bis(2-Hydroxyethyl)amino]azobenzene

4-[bis(2-Hydroxyethyl)amino]azobenzene

RN: 2452-84-8 MP (°C): 134

MW: 285.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-04	3.139E-02	25	B333	0 0 0 0 0	

3640. C₁₆H₁₉N₃O₄S

Cephradine

Anspor

Velosef

RN: 38821-53-3 MP (°C): 140

MW: 349.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.096E-02	2.130E+01	ns	F181	0 0 0 0 2	

3641. C₁₆H₁₉N₃O₄S

Ampicillin

(2S,5R,6R)-6-[(R)-2-Amino-2-phenylacetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid

Aminobenzylpenicillin

Unasyn

Wymox

Totacillin

RN: 69-53-4**MP (°C):****MW:** 349.41**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.293E-02	1.500E+01	7.5	P009	1 0 2 1 0	EFG
3.721E-02	1.300E+01	20	P009	1 0 2 1 0	EFG
2.890E-02	1.010E+01	21	M044	2 0 2 2 2	
3.978E-02	1.390E+01	25	H051	1 2 2 2 2	
6.600E-03	2.306E+00	25	K444	0 0 0 0 0	
3.434E-02	1.200E+01	30	P009	1 0 2 1 0	EFG
3.291E-02	1.150E+01	40	P009	1 0 2 1 0	EFG

3642. C₁₆H₁₉N₃O₄S.3H₂O

Ampicillin (trihydrate)

RN: 7177-48-2**MP (°C):** 198**MW:** 403.46**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-02	5.700E+00	7.5	P009	1 0 2 1 0	EFG
1.487E-02	6.000E+00	20	P009	1 0 2 1 0	EFG
1.873E-02	7.558E+00	21	M044	2 0 2 2 2	
1.983E-02	8.000E+00	30	P009	1 0 2 1 0	EFG
2.479E-02	1.000E+01	40	P009	1 0 2 1 0	EFG

3643. C₁₆H₁₉N₃O₅S

Amoxicillin

RN: 61336-70-7**MP (°C):****MW:** 365.41**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.095E-02	4.000E+00	ns	K444	0 0 0 0 0	

3644. C₁₆H₁₉N₃O₅S.3H₂O

Amoxicillin (trihydrate)

4-Thia-1-azabicyclo(3.2.0)heptane-2-carboxylic acid (trihydrate)

RN: 61336-70-7 MP (°C):

MW: 419.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~9.54E-03	~4.00E+00	ns	B188	0 0 0 0 0	

3645. C₁₆H₁₉N₅O

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 2-dimethylamino)-11-ethyl-5,11-dihydro-4-methyl-

RN: 135795-08-3 MP (°C):

MW: 297.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.346E-05	4.002E-03	ns	M381	0 1 1 1 2	pH 7.0

3646. C₁₆H₁₉N₅O₂

6H-Dipyrido[3,2-b:2',3'-e][1,4]diazepin-6-one, 11-ethyl-5,11-dihydro-2-[(2-hydroxyethyl)methylamino]

RN: 155206-46-5 MP (°C):

MW: 313.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.365E-04	1.368E-01	ns	M381	0 1 1 1 2	pH 7.0

3647. C₁₆H₁₉O₄P

Butyl diphenyl phosphate

RN: 2752-95-6 MP (°C):

MW: 306.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.53E-04	<2.00E-01	25	B070	1 2 0 1 0	

3648. C₁₆H₂₀I₃N₃O₇

1,3-Benzenedicarboxamide, N-(2-hydroxyethyl)-N'-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (S)-

RN: 77868-44-1 MP (°C):

MW: 747.07 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.625E-02	1.961E+01	25	P091	0 0 0 0 0	

3649. C₁₆H₂₀I₃N₃O₇

1,3-Benzenedicarboxamide, *N*-(2,3-dihydroxypropyl)-*N'*-(2-hydroxyethyl)-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-(RS)

RN: 77868-43-0 **MP (°C):**
MW: 747.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.374E-02	4.762E+01	25	P091	0 0 0 0 0	

3650. C₁₆H₂₀I₃N₃O₈

1,3-Benzenedicarboxamide, *N,N'*-bis(2,3-dihydroxypropyl)-5*S*-[(hydroxyacetyl)amino]-2,4,6-triiodo- [RS-(RS*,RS*)]-

RN: 77868-40-7 **MP (°C):**
MW: 763.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.317E-02	1.768E+01	25	P091	0 0 0 0 0	

3651. C₁₆H₂₀I₃N₃O₈

1,3-Benzenedicarboxamide, 5-[(hydroxyacetyl)amino]-*N,N'*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 77868-41-8 **MP (°C):**
MW: 763.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.282E-02	4.031E+01	25	P091	0 0 0 0 0	

3652. C₁₆H₂₀N₄O₂

Apazone

APZ

Azapropazone

RN: 13539-59-8 **MP (°C):** 247
MW: 300.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-04	1.472E-01	35	H091	1 2 2 2 1	<i>sic</i>
2.896E-04	8.700E-02	rt	H302	0 0 2 1 1	intrinsic

3653. C₁₆H₂₀N₄O₃S

2-(*N*4-Acetylsulfanilylamoно)-4-isobutylpyrimidine

RN: **MP (°C):**
MW: 348.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.091E-05	3.800E-03	37	R076	1 2 0 0 1	

3654. C₁₆H₂₀N₈O₂S

6-[D-2-Amino-2-(4-aminophenyl)-acetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]hept-2-yl-5-t

RN: MP (°C):
MW: 388.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.277E-03	2.050E+00	25	B148	2 2 2 1 2	

3655. C₁₆H₂₀O₆P₂S₃

Temephos

O,O'-(Thiodi-4,1-phenylene)bis(*O,O'*-dimethylphosphorothioate)

Abate

Tetramethyl *O,O'*-thiodi-*p*-phenylene phosphorothioate

Abaphos

Tetrafenphos

RN: 3383-96-8 MP (°C):
MW: 466.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.929E-08	9.000E-06	10	B324	0 0 0 0 0	
1.929E-08	8.998E-06	10	B324	0 0 0 0 0	
5.788E-07	2.700E-04	20	B300	2 1 1 1 2	
5.788E-07	2.700E-04	20	B324	0 0 0 0 0	
5.788E-07	2.700E-04	20	B324	0 0 0 0 0	
1.501E-06	7.002E-04	30	B324	0 0 0 0 0	
1.501E-06	7.000E-04	30	B324	0 0 0 0 0	

3656. C₁₆H₂₁CIN₃S

Methylene blue

Methylenblau

C.I. 52015

RN: 61-73-4 MP (°C):
MW: 322.88 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.02E-01	~3.30E+01	20	F300	1 0 0 0 0	

3657. C₁₆H₂₁NO

N,N-Heptamethylenecinnamamide

Octahydro-1-(1-oxo-3-phenyl-2-propenyl) azocine

RN: 59832-06-3 MP (°C):
MW: 243.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-04	6.230E-02	ns	H350	0 0 0 0 0	

3658. C₁₆H₂₁NO*N*-Cycloheptylcinnamamide*N*-Cycloheptyl-3-phenyl-2-propenamide

RN: 59831-98-0 MP (°C):

MW: 243.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.570E-06	8.688E-04	ns	H350	0 0 0 0 0	

3659. C₁₆H₂₁NO₂

Propranolol

2-Propanol, 1-[(1-methylethyl)amino]-3-(1-naphthalenyloxy)-

RN: 525-66-6 MP (°C):

MW: 259.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.195E-04	3.100E-02	22.5	B422	0 0 0 0 0	
3.123E-04	8.099E-02	25	S450	0 0 0 0 0	
3.092E-08	8.020E-06	32	M458	0 0 0 0 0	

3660. C₁₆H₂₁NO₂S*m*-Carboxyloctylphenylisothiocyanate

3-Carboxyloctylphenylisothiocyanate

RN: MP (°C):

MW: 291.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.748E-02	25	K032	2 2 0 1 1	

3661. C₁₆H₂₁NO₃

Piperidine, 1-[(benzoyloxy)acetyl]-2-ethyl-

RN: 115178-69-3 MP (°C): 54.5

MW: 275.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.889E-03	5.200E-01	22	N317	1 1 2 1 2	

3662. C₁₆H₂₁NO₃

Piperidine, 1-[(benzoyloxy)acetyl]-2,6-dimethyl-

RN: 115178-70-6 MP (°C): 118

MW: 275.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.448E-04	1.500E-01	22	N317	1 1 2 1 2	

3663. C₁₆H₂₁NO₃Acetamide, 2-(benzoyloxy)-*N*-cyclohexyl-*N*-methyl-**RN:** 106231-65-6 **MP (°C):****MW:** 275.35 **BP (°C):** 439.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.084E-04	1.400E-01	22	B427	1 0 0 1 1	

3664. C₁₆H₂₁NO₅

Benzoic acid, 2-(acetyloxy)-, 2-(diethylamino)-1-methyl-2-oxoethyl ester

RN: 118247-09-9 **MP (°C):** 40.5**MW:** 307.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.499E-02	7.680E+00	21	N335	0 0 0 0 0	

3665. C₁₆H₂₁N₃

Tripeleannamine

N-Benzyl-*N'*,*N'*-dimethyl-*N*-2-pyridylethylenediamine

PBZ

Pelamine

RN: 91-81-6 **MP (°C):** <25**MW:** 255.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	5.873E-01	30	L068	1 0 0 1 0	EFG
1.500E-02	3.830E+00	37.5	L034	2 2 0 1 2	pH 7.4

3666. C₁₆H₂₂Cl₂O₃2,4-Dichlorophenoxyacetic acid *n*-octyl ester

2,4-Dichlorophenoxyacetic acid capryl ester

RN: 1928-44-5 **MP (°C):****MW:** 333.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.128E-05	7.092E-03	ns	M120	0 0 1 1 2	

3667. C₁₆H₂₂N₄O

Neohetramine

N,N-Dimethyl-N'-(*p*-methoxybenzyl)-N'-(2-pyrimidyl)ethylenediamine

Tonzilamine

RN: 91-85-0**MP (°C):****MW:** 286.38**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-02	5.441E+00	37.5	L034	2 2 0 1 2	pH 7.4

3668. C₁₆H₂₂N₄O₂S2-Sulfanilamido-4-methyl-5-*n*-amylpyrimidine**RN:** 71119-35-2 **MP (°C):** 188-190**MW:** 334.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.372E-05	2.800E-02	29	C049	0 0 0 0 0	

3669. C₁₆H₂₂N₄O₆

2'-Valeryl-6-methoxypurine arabinoside

2'-Trimethylacetyl-6-methoxypurine arabinoside

RN: 121032-22-2 **MP (°C):** 118-120**MW:** 366.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-01	8.793E+01	37	C348	0 0 0 0 0	pH 7.00
1.070E-01	3.920E+01	37	C348	0 0 0 0 0	pH 7.00

3670. C₁₆H₂₂N₄O₆.0.5H₂O6-Methoxy-9-(5-*O*-pivalate-β-D-arabinofuranosyl)]-9H-purine (hemihydrate)**RN:** 121032-42-6 **MP (°C):** glass**MW:** 375.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.560E-02	1.336E+01	37	M378	1 2 1 1 2	pH 7.2

3671. C₁₆H₂₂N₄O₆.0.5H₂O6-Methoxy-9-(5-*O*-valerate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)**RN:** 142963-77-7 **MP (°C):** foam**MW:** 375.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.720E-03	6.457E-01	37	M378	1 2 1 1 2	pH 7.2

3672. C₁₆H₂₂O₄

Dibutyl phthalate

n-Butyl phthalate

RN: 84-74-2

MP (°C): -35

MW: 278.35

BP (°C): 430

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.455E-05	1.240E-02	10	S198	2 1 2 2 2	
3.952E-05	1.100E-02	15	H069	1 0 1 1 1	
3.630E-05	1.010E-02	20	L300	2 1 0 2 2	
3.880E-05	1.080E-02	20	S198	2 1 2 2 2	
3.593E-04	1.000E-01	22	N311	1 0 1 1 2	
3.377E-05	9.400E-03	22	Y419	0 0 0 0 0	
6.574E-05	1.830E-02	23.5	S171	2 1 2 2 2	
3.126E-05	8.700E-03	25	D336	0 0 0 0 0	
3.449E-05	9.600E-03	25	D336	0 0 0 0 0	
4.670E-05	1.300E-02	25	F067	1 0 2 2 2	
1.609E-02	4.480E+00	25	F070	1 0 0 0 2	<i>sic</i>
4.095E-05	1.140E-02	30	S198	2 1 2 2 2	
1.437E-03	4.000E-01	rt	M161	0 0 0 0 2	

3673. C₁₆H₂₂O₄

Diisobutyl phthalate

1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) esterpalatinol

Phthalic acid diisobutyl ester

Palatinolic

RN: 84-69-5

MP (°C):

MW: 278.35

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.592E-04	9.999E-02	20	F070	1 0 0 0 2	
7.300E-05	2.032E-02	20	L300	2 1 0 2 2	
2.227E-05	6.200E-03	24	H116	2 1 0 0 2	
5.030E-06	1.400E-03	25	D336	0 0 0 0 0	

3674. C₁₆H₂₂O₄*tert*-Butyl phthalate

RN: 30448-43-2 MP (°C):

MW: 278.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.952E-06	1.100E-03	25	D336	0 0 0 0 0	

3675. C₁₆H₂₂O₄Di-*n*-butyl *o*-phthalate

RN: **MP (°C):** -35 C
MW: 278.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.593E-05	1.000E-02	25	S417	0 0 0 0 0	

3676. C₁₆H₂₂O₆Diethoxyethyl phthalate
bis(2-Ethoxyethyl) phthalate

RN: 605-54-9 **MP (°C):**
MW: 310.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.271E-03	1.946E+00	ns	F014	0 0 0 0 2	

3677. C₁₆H₂₂O₈.2H₂O

Coniferin (dihydrate)

4-Hydroxy-3-methoxy-1-(γ -hydroxypropenyl)benzene-4-D-glucoside (dihydrate)

Abietin(dihydrate)

Coniferosi(dihydrate)

RN: 531-29-3 **MP (°C):** 185
MW: 378.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.315E-02	4.975E+00	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

3678. C₁₆H₂₂O₁₁ β -D-Glucose pentaacetate β -Glucose-penta-acetat

RN: 604-69-3 **MP (°C):** 131
MW: 390.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.306E-03	9.000E-01	18	F300	1 0 0 0 0	

3679. C₁₆H₂₂O₁₁ α -D-Glucose pentaacetate1,2,3,4,6-Penta-O-acetyl- α -D-glucose

Pentaacetate

Glucopyranose pentaacetate

Glucose pentaacetate;

 α -D-Glucopyranose

RN: 604-68-2 MP (°C): 109–111

MW: 390.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.802E-03	1.484E+00	ns	R427	0 0 0 0 0	

3680. C₁₆H₂₂O₁₁ α -Glucose pentaacetate α -Glucosid-penta-acetat

RN: 3891-59-6 MP (°C): 110

MW: 390.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.843E-03	1.500E+00	18	F300	1 0 0 0 1	

3681. C₁₆H₂₃FN₂O₆

1,3-bis(Pivaloyloxymethyl)-5-fluoro-2,4(1H,3H)-pyrimidinedi-one

1,3-bis(Pivaloyloxymethyl)-5-fluorouracil

RN: 66542-50-5 MP (°C): 102–104

MW: 358.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.256E-04	4.500E-02	22	B321	0 0 0 0 0	pH 4.0

3682. C₁₆H₂₃NO*n*-Heptylcinnamamide2-Propenamide, *N*-heptyl-3-phenyl-

RN: 59831-99-1 MP (°C):

MW: 245.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-06	1.865E-03	ns	H350	0 0 0 0 0	

3683. C₁₆H₂₃NO₂

Etoxadrol

(+)-2-(2-Ethyl-2-phenyl-1,3-dioxolan-4-yl)piperidine

RN: 28189-85-7 MP (°C):

MW: 261.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.487E-03	6.500E-01	20	K017	1 2 2 2 2	pH 10, intrinsic
1.098E-02	2.870E+00	30	K017	1 2 2 2 2	pH 10, intrinsic
4.668E-02	1.220E+01	40	K017	1 2 2 2 2	pH 10, intrinsic

3684. C₁₆H₂₃NO₃

Acetaminophen octanoate

Octanoic acid, 4-(acetylamino)phenyl ester

RN: 54942-41-5 MP (°C): 103

MW: 277.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.605E-05	1.000E-02	25	B010	1 1 1 1 0	

3685. C₁₆H₂₃NO₃S₂N-[2-(3,4-Dihydroxyphenyl)ethyl]-5-[(3*R*)-1,2-dithiolan-3-yl]-pentanamide

RN: MP (°C):

MW: 341.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.054E-06	3.600E-04	ns	S453	0 0 0 0 0	

3686. C₁₆H₂₃NO₆

Monocrotaline

(-)-Monocrotaline

RN: 315-22-0 MP (°C): 202

MW: 325.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.644E-02	1.186E+01	ns	I312	0 0 0 0 0	

3687. C₁₆H₂₃N₅O₅

9-[5'-(O-Caproyl)-β-D-arabinofuranosyl]adenine ester

RN: 65926-34-3 MP (°C):

MW: 365.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.842E-03	2.500E+00	ns	B134	0 1 1 1 1	

3688. C₁₆H₂₃N₅O₅9-[5'-(*O*-*tert*-Butylacetyl)- β -D-arabinofuranosyl]adenine ester**RN:** 68325-42-8 **MP (°C):****MW:** 365.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.135E-02	7.800E+00	ns	B134	0 1 1 1 1	

3689. C₁₆H₂₄N₂O₂*N,N,N',N'*-Tetraethylterephthalamide**RN:** 15394-30-6 **MP (°C):****MW:** 276.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-02	5.528E+00	30	K019	1 0 0 0 1	

3690. C₁₆H₂₄N₂O₂*N,N,N',N'*-Tetraethylisophthalamide**RN:** 13698-87-8 **MP (°C):****MW:** 276.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-01	1.990E+02	30	K019	1 0 0 0 2	

3691. C₁₆H₂₄N₄O₂

2,5-Diaziridinyl-3,6-bis(propylamino)-1,4-benzoquinone

RN: 59886-47-4 **MP (°C):** 140**MW:** 304.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.29E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3692. C₁₆H₂₄N₄O₆

2,5-Diaziridinyl-3,6-bis(2'-hydroxyl-3'-hydroxylpropylamino)-1,4-benzoquinone

2,5-Diaziridinyl-3,6-bis(hydroxylethylmethylamino)-1,4-benzoquinone

RN: 59886-55-4 **MP (°C):** 273**MW:** 368.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.629E-01	6.000E+01	rt	C317	0 0 0 0 0	
8.143E-02	3.000E+01	rt	C317	0 0 0 0 0	

3693. C₁₆H₂₄N₆1-(Methylphenethylamino)-3,5-bis(dimethylamino)-*s*-triazine

RN: 125867-93-8 MP (°C):

MW: 300.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.427E-05	7.291E-03	25	B386	0 0 0 0 0	

3694. C₁₆H₂₄O₃Nonyl *p*-hydroxybenzoate

Nonyl 4-hydroxybenzoate

RN: 38713-56-3 MP (°C):

MW: 264.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.824E-03	1.275E+00	25	D081	1 2 2 1 2	

3695. C₁₆H₂₄O₄

3,4-Epoxy-6-methylcyclohexylmethyl-3,4-epoxy-6-methylcyclohexane carboxylate

EP 201

RN: 141-37-7 MP (°C):

MW: 280.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.067E-02	2.991E+00	ns	I313	0 0 0 0 0	

3696. C₁₆H₂₅NOSS-Benzyl di-*sec*-butylthiocarbamate

Thiocarbazil

Tiocarbazil

RN: 36756-79-3 MP (°C):

MW: 279.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.946E-06	2.500E-03	30	M161	1 0 0 0 1	

3697. C₁₆H₂₅NO₂

Butacarb

Carbamic acid, *N*-methyl-, 3,5-di-*tert*-butylphenyl ester3,5-Di-*tert*-butylphenyl methylcarbamate**RN:** 2655-19-8 **MP (°C):** 102.9**MW:** 263.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.695E-05	1.500E-02	20	M161	1 0 0 0 1	

3698. C₁₆H₂₅NO₂Nonyl *p*-aminobenzoate

Nonyl 4-aminobenzoate

RN: 37139-21-2 **MP (°C):****MW:** 263.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.020E-06	2.687E-04	37	F006	1 1 2 2 2	

3699. C₁₆H₂₅NO₃

4-Propoxybenzoic acid-2-(diethyl-amino)ethyl ester

RN: 15788-85-9 **MP (°C):****MW:** 279.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-04	1.257E-01	ns	M066	0 0 0 0 1	

3700. C₁₆H₂₆

2-Phenyldecane

RN: **MP (°C):****MW:** 218.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.600E-08	5.678E-06	25	S377	0 0 0 0 0	

3701. C₁₆H₂₆

3-Phenyldecane

RN: **MP (°C):****MW:** 218.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	8.299E-06	25	S377	0 0 0 0 0	

3702. C₁₆H₂₆

4-Phenyldecane

RN:**MW:** 218.39**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-08	7.862E-06	25	S377	0 0 0 0 0	

3703. C₁₆H₂₆

5-Phenyldecane

RN:**MW:** 218.39**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-08	7.643E-06	25	S377	0 0 0 0 0	

3704. C₁₆H₂₆N₂O₂

4-Propylaminobenzoic acid-2-(diethyl-amino)ethyl ester

RN: 16488-54-3 **MP (°C):****MW:** 278.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-03	2.867E-01	ns	M066	0 0 0 0 2	

3705. C₁₆H₂₆O₂

4-Octylphenol monoethoxylate

RN: 51437-89-9 **MP (°C):****MW:** 250.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.195E-05	8.000E-03	20.5	A335	0 0 0 0 0	
3.200E-05	8.012E-03	20.5	A335	0 0 0 0 0	

3706. C₁₆H₂₆O₅

Artemether

RN: 71963-77-4 **MP (°C):****MW:** 298.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
		ns	K444	0 0 0 0 0	

3707. C₁₆H₂₆O₆

Triethylene glycol dibutyrate

RN: 26962-26-5 **MP (°C):**
MW: 314.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.524E-02	7.937E+00	ns	F014	0 0 0 0 2	

3708. C₁₆H₂₈N₃O₂

Dioxyethylaminoazobenzene

RN: **MP (°C):**
MW: 294.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.945E-04	8.670E-02	0	K036	1 0 0 0 2	
4.212E-04	1.240E-01	25	K036	1 0 0 0 2	
2.819E-03	8.300E-01	90	K036	1 0 0 0 2	

3709. C₁₆H₃₂O₂

Palmitic acid

Hexadecanoic acid

RN: 57-10-3 **MP (°C):** 56
MW: 256.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.794E-05	4.600E-03	0	B136	1 0 2 1 1	
2.808E-05	7.200E-03	20	B136	1 0 2 1 1	
2.808E-05	7.200E-03	20.0	R001	1 1 1 1 1	
3.200E-06	8.206E-04	25	J001	1 0 2 1 1	
1.200E-07	3.077E-05	25	R002	0 0 0 0 0	intrinsic
2.680E-06	6.872E-04	25	R002	0 0 0 0 0	
3.237E-05	8.300E-03	30	B136	1 0 2 1 1	
3.237E-05	8.300E-03	30.0	R001	1 1 1 1 1	
3.900E-05	1.000E-02	45	B136	1 0 2 1 1	
3.900E-05	1.000E-02	45.0	R001	1 1 1 1 1	
4.000E-06	1.026E-03	50	J001	1 0 2 1 1	
4.680E-05	1.200E-02	60	B136	1 0 2 1 1	
4.680E-05	1.200E-02	60.0	R001	1 1 1 1 1	
1.794E-05	4.600E-03	.0	R001	1 1 1 1 1	

3710. C₁₆H₃₄

2,2,4,4,6,8,8-Heptamethylnonane

RN: 4390-04-9 **MP (°C):**
MW: 226.45 **BP (°C):** 240

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.369E-09	3.100E-07	25	T423	0 0 0 0 0	

3711. C₁₆H₃₄

3-Methylpentadecane

RN: 2882-96-4 **MP (°C):** -22
MW: 226.45 **BP (°C):** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.328E-10	9.800E-08	23	C332	0 0 0 0 0	

3712. C₁₆H₃₄

Hexadecane

n-Hexadecane

Cetane

RN: 544-76-3 **MP (°C):** 18.17
MW: 226.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.778E-08	6.290E-06	25	F004	0 0 0 0 0	

3713. C₁₆H₃₄

2-Methylpentadecane

RN: 1560-93-6 **MP (°C):** -7
MW: 226.45 **BP (°C):** 282

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.681E-10	1.060E-07	23	C332	0 0 0 0 0	

3714. C₁₆H₃₄O

Hexadecanol

Cetyl alcohol

RN: 36653-82-4 **MP (°C):** 49
MW: 242.45 **BP (°C):** 344

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.699E-07	4.120E-05	22.5	G301	0 0 0 0 0	
1.700E-07	4.122E-05	25	R002	0 0 0 0 0	
3.300E-08	8.001E-06	34	K011	1 2 1 1 2	

(continued)

3714. C₁₆H₃₄O (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.393E-08	1.550E-05	43	H030	2 2 2 2 2	
6.393E-08	1.550E-05	43	H103	1 2 2 2 2	
1.270E-07	3.079E-05	55	K011	1 2 1 1 2	
1.675E-07	4.060E-05	61	H030	2 2 2 2 2	
1.675E-07	4.060E-05	61	H103	1 2 2 2 2	

3715. C₁₆H₃₅O₃P

Dibutyl isoocetyl phosphonate

RN: 108979-58-4 MP (°C):

MW: 306.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.53E-04	<2.00E-01	25	B070	1 2 0 1 0	

3716. C₁₆H₃₅O₄P

Dibutyl octyl phosphate

RN: 25786-28-1 MP (°C):

MW: 322.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.10E-04	<1.00E-01	25	B070	1 2 0 1 0	

3717. C₁₇H₁₁NO₃

Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-1-phenyl-

RN: 74103-09-6 MP (°C):

MW: 277.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.190E-07	3.300E-05	25	P089	0 0 0 0 0	
1.388E-07	3.850E-05	37	P089	0 0 0 0 0	
1.677E-07	4.650E-05	51	P089	0 0 0 0 0	

3718. C₁₇H₁₂

1,2-Benzofluorene

Benzo[a]fluorene

11H-Benzo[a]fluorene

RN: 238-84-6 MP (°C): 187

MW: 216.29 BP (°C): 407

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.081E-07	4.500E-05	25	M064	1 1 2 2 1	
2.100E-07	4.542E-05	25	M342	1 0 1 1 1	
2.081E-07	4.500E-05	ns	M344	0 0 0 0 2	

3719. C₁₇H₁₂

2,3-Benzofluorene

Benzo[b]fluorene

11H-Benzo[b]fluorene

RN: 243-17-4**MP (°C):** 209**MW:** 216.29**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.849E-08	4.000E-06	25	B319	2 0 1 2 0	
9.247E-09	2.000E-06	25	M064	1 1 2 2 1	
9.250E-09	2.001E-06	25	M342	1 0 1 1 2	

3720. C₁₇H₁₂CIFN₂O

Nuarimol

Triminol

Trimidal

Gauntlet

2-Chloro-4'-fluoro- α -(5-pyrimidinyl)benzhydryl alcohol α -(2-Chlorophenyl)- α -(4-fluorophenyl)-5-pyrimidinemethanol**RN:** 63284-71-9**MP (°C):****MW:** 314.75**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-05	2.618E-02	ns	R427	0 0 0 0 0	

3721. C₁₇H₁₂CIFN₃O₂ α -(4-Chlorophenyl)- α -(1-2-(2-chloro)phenylethenyl)-1H-1,2,4-triazole-1-ethanol

X-7801

DuP 860

RN:**MP (°C):****MW:** 344.76**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.612E-06	1.590E-03	22	M362	1 1 2 1 1	

3722. C₁₇H₁₂CINO₂S

Fentiazac

4-(*p*-Chlorophenyl)-2-phenyl-5-thiazoleacetic acid**RN:** 18046-21-4**MP (°C):** 161.1**MW:** 329.81**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-06	3.100E-03	5	F306	1 0 1 2 2	
9.600E-05	3.166E-02	25	C314	0 0 0 0 0	
9.612E-05	3.170E-02	25	C314	0 0 0 0 0	intrinsic

(continued)

3722. C₁₇H₁₂CINO₂S (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.080E-05	3.562E-03	25	F306	1 0 1 2 2	intrinsic
1.310E-05	4.320E-03	37	F306	1 0 1 2 2	intrinsic
1.072E-05	3.534E-03	ns	R427	0 0 0 0 0	

3723. C₁₇H₁₂Cl₂N₂O

Fenarimol

2,4'-Dichloro- α -(5-pyrimidinyl)benzhydryl alcohol α -(2-Chlorophenyl)- α -(4-chlorophenyl)-5-pyrimidinemethanol

Tebulan

Rubigan 4AS

Rimidin

RN: 60168-88-9 MP (°C): 118

MW: 331.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.136E-05	1.370E-02	25	M161	1 0 0 0 2	pH 7

3724. C₁₇H₁₂Cl₂N₄

Triazolam

8-Chloro-6-(*o*-chlorophenyl)-1-methyl-4H-s-triazolo[4,3-a][1,4]benzodiazepine

Apo-Triazo

Gen-Triazolam

Halcion

Novo-Triolam

RN: 28911-01-5 MP (°C):

MW: 343.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.741E-05	3.000E-02	amb	L434	0 0 0 0 0	

3725. C₁₇H₁₂Cl₁₀O₃

Kelevan

Allied GC 9160

Despirol

RN: 4234-79-1 MP (°C): 91

MW: 618.81 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.888E-06	5.500E-03	20	M164	1 0 0 0 1	

3726. C₁₇H₁₂I₂O₃

Benziodarone

Algocor

Amplivix

Dilafurane

RN: 68-90-6**MP (°C):****MW:** 518.09**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-05	5.881E-03	20	H301	0 0 0 0 0	

3727. C₁₇H₁₂O₆

Aflatoxin B1

AFB1

RN: 1162-65-8**MP (°C):** 268**MW:** 312.28**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.803E-05	1.500E-02	ns	I306	0 0 0 0 0	

3728. C₁₇H₁₂O₇

Aflatoxin G1

RN: 1165-39-5**MP (°C):** 244**MW:** 328.28**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.569E-05	1.500E-02	ns	I306	0 0 0 0 0	

3729. C₁₇H₁₃ClN₄

Alprazolam

8-Chloro-1-methyl-6-phenyl-4H-s-triazolo[4,3-a][1,4]benzodiazepine

Apo-Alpraz

Kalma

Novo-Alprazol

Nu-Alpraz

RN: 28981-97-7**MP (°C):****MW:** 308.77**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.267E-04	7.000E-02	amb	L434	0 0 0 0 0	
3.239E-04	1.000E-01	amb	L445	0 0 0 0 0	intrinsic

3730. C₁₇H₁₃ClO₃

Itanoxone

2'-Chloro- α -methylene- γ -oxo[1,1'-biphenyl]-4-butanoic acid

F 1379

RN: 58182-63-1 **MP (°C):** 212**MW:** 300.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.318E-04	1.900E-01	20	C112	2 0 1 1 2	

3731. C₁₇H₁₃Cl₂N₃O₂ α -(2,4-Difluorophenyl)- α -(1-2-(2-chloro)phenylethenyl)-1H-1,2,4-triazole-1-ethanol

A-9991

DuP 991

RN: **MP (°C):**
MW: 362.22 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.933E-05	7.000E-03	22	M362	1 1 2 1 1	

3732. C₁₇H₁₄F₃N₃O₂S

Celecoxib

4-[5-(4-Methylphenyl)-3-(trifluoromethyl)

Celebrex

SC-58635

YM-177

RN: 169590-42-5 **MP (°C):**
MW: 381.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.835E-05	7.000E-03	25	S415	0 0 0 0 0	
7.866E-06	3.000E-03	37	Y412	0 0 0 0 0	

3733. C₁₇H₁₄N₂O1-*o*-Tolylazo-2-naphthol

Orange OT

Oil orange SS

1-(*o*-Tolylazo)-2-naphthol**RN:** 2646-17-5 **MP (°C):** 131
MW: 262.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.624E-07	2.000E-04	30	R430	0 0 0 0 0	
1.000E-07	2.623E-05	rt	M163	0 0 0 0 1	

3734. C₁₇H₁₄O₄S

Rofecoxib

4-(4-Methylsulfonylphenyl)-3-phenyl-5H-furan-2-one

RN: 162011-90-7 MP (°C):

MW: 314.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.605E-05	8.190E-03	24.99	D414	0 0 0 0 0	
2.863E-05	9.000E-03	25	S415	0 0 0 0 0	
2.977E-05	9.360E-03	29.99	D414	0 0 0 0 0	
3.556E-05	1.118E-02	34.99	D414	0 0 0 0 0	
2.545E-06	8.000E-04	37	Y421	0 0 0 0 0	

3735. C₁₇H₁₄O₆

Aflatoxin B2

RN: 7220-81-7 MP (°C): 286

MW: 314.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.773E-05	1.500E-02	ns	I306	0 0 0 0 0	

3736. C₁₇H₁₄O₇

Aflatoxin G2

RN: 7241-98-7 MP (°C): 237

MW: 330.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.541E-05	1.500E-02	ns	I306	0 0 0 0 0	

3737. C₁₇H₁₅NO₃

Cinnamyl acetaminophen

Cinnamic acid, ester with 4'-hydroxyacetanilide

Acetanilide, 4'-hydroxy-, cinnamate (ester)

RN: 20682-28-4 MP (°C): 200–201

MW: 281.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.977E-06	1.400E-03	37	D029	0 0 0 0 0	

3738. C₁₇H₁₅NO₅

Benzoic acid, 2-(acetoxy)-, 4-(acetylamino)phenyl ester

RN: 5003-48-5 MP (°C): 174.5

MW: 313.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.383E-05	2.000E-02	21	N335	0 0 0 0 0	

3739. C₁₇H₁₆Br₂O₃

Bromopropylate

1-Methylethyl-4-bromo- α -(4-bromophenyl)- α -hydroxybenzeneacetate

Neoron

GS-19851

Phenisobromolate

RN: 18181-80-1 MP (°C): 77

MW: 428.13 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.17E-06	<5.00E-04	20	F311	1 2 2 2 1	
1.168E-05	5.000E-03	20	M161	1 0 0 0 0	

3740. C₁₇H₁₆CIFN₂O₂

Progabide

Butanamide, 4-[[[4-chlorophenyl)(5-fluoro-2-hydroxyphenyl)methylene]amino]-

Gabrene

SL 76-002

RN: 62666-20-0 MP (°C):

MW: 334.78 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.110E-04	3.716E-02	37	F309	1 0 2 2 2	
1.110E-04	3.716E-02	37	F318	2 2 0 0 2	

3741. C₁₇H₁₆Cl₂O₃

Chloropropylate

1-Methylethyl-4-chloro- α -(4-chlorophenyl)- α -hydroxybenzenacetate

Chlormite

Acaralate

G-24163

Rospin

RN: 5836-10-2 MP (°C): 74

MW: 339.22 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.422E-06	1.500E-03	20	F311	1 2 2 2 1	
2.948E-05	1.000E-02	rt	M161	0 0 0 0 1	

3742. C₁₇H₁₆N₂O₂S

1-Sulfamethylnaphthalene

RN: MP (°C):
MW: 312.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.201E-05	1.000E-02	20	F073	1 2 2 2 1	

3743. C₁₇H₁₆N₂O₃

C.I. Disperse blue 3

1-[(2-Hydroxyethyl)amino]-4-(methylamino)-9,10-anthracenedione

C.I. 61505

RN: 2475-46-9 MP (°C): 187
MW: 296.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-07	3.556E-05	25	B333	0 0 0 0 0	

3744. C₁₇H₁₆N₂O₃S

4-Sulfahydroxymethylnaphthalene

RN: MP (°C):
MW: 328.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-04	5.500E-02	20	F073	1 2 2 2 1	

3745. C₁₇H₁₆N₂O₄

p-(p-Acetamidobenzamido)phenyl acetate

RN: 74973-19-6 MP (°C):
MW: 312.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-05	1.218E-02	25	A066	1 0 1 1 1	

3746. C₁₇H₁₆N₂O₄S

1-Benzenesulfonyl-5-ethyl-5-phenyl-hydantoin

5-Ethyl-5-phenyl-1(phenylsulfonyl)-2,4-imidazolidinedione

RN: 21413-25-2 MP (°C):
MW: 344.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.782E-04	3.369E-01	37	F183	1 0 1 1 1	intrinsic

3747. C₁₇H₁₆N₂O₅

p-4-Acetaminophenyl acetaminophen
 Acetamide, *N,N'*-[carbonylbis(oxy-4,1-phenylene)]bis-
 Acetanilide, 4'-hydroxy-, carbonate (2:1) (ester)

RN: 19872-72-1 **MP (°C):** 219.5–220
MW: 328.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.827E-04	6.000E-02	37	D029	0 0 0 0 0	

3748. C₁₇H₁₇ClO₆

Griseofulvin

(2*S-trans*)-7-Chloro-2',4,6-trimethoxy-6'-methylspiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4'-dione

Fulvicin

Grisactin

Grifulvin

Griseostatin

RN: 126-07-8 **MP (°C):** 220.0
MW: 352.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.830E-05	6.456E-03	15	E010	2 2 2 2 2	
2.466E-05	8.700E-03	20	N322	0 0 0 0 0	
3.260E-05	1.150E-02	21	E316	0 0 0 0 0	
3.175E-04	1.120E-01	21	M044	2 0 2 2 2	<i>sic</i>
4.025E-04	1.420E-01	21	M044	2 0 2 2 2	microsize, <i>sic</i>
2.126E-05	7.500E-03	22	C040	2 0 2 2 0	EFG
2.076E-05	7.325E-03	22	M382	2 1 1 1 1	average of 2
1.474E-05	5.200E-03	22.5	B422	2 0 2 2 2	
2.523E-05	8.900E-03	23	B362	0 0 0 0 0	
2.268E-05	8.000E-03	25	C037	2 1 2 2 2	
2.450E-05	8.643E-03	25	E010	2 2 2 2 2	
3.685E-05	1.300E-02	25	H015	1 0 0 0 1	
2.835E-05	1.000E-02	25	L033	1 0 2 1 1	
2.268E-05	8.000E-03	25	M457	0 0 0 0 0	
2.750E-05	9.700E-03	25	P096	0 0 0 0 0	
2.551E-05	9.000E-03	27	B043	1 0 1 2 0	EFG
2.835E-05	1.000E-02	30	M045	2 0 0 0 0	
4.000E-05	1.411E-02	30	O321	0 0 0 0 0	
4.252E-05	1.500E-02	30	O321	0 0 0 0 0	
3.510E-05	1.238E-02	35	E010	2 2 2 2 2	
3.969E-05	1.400E-02	37	B039	2 1 1 1 0	EFG
4.252E-05	1.500E-02	37	B043	1 0 1 2 0	EFG
3.969E-05	1.400E-02	37	B045	1 0 1 1 1	
4.054E-05	1.430E-02	37	F033	2 0 2 0 2	
3.968E-05	1.400E-02	37	G011	1 0 1 1 0	EFG
4.252E-05	1.500E-02	37	K018	1 0 0 0 1	
5.669E-05	2.000E-02	45	B043	1 0 1 2 0	EFG (continued)

3748. C₁₇H₁₇ClO₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.140E-05	2.166E-02	45	E010	2 2 2 2 2	
3.798E-05	1.340E-02	ns	D340	0 0 0 0 0	
2.835E-04	1.000E-01	ns	K444	0 0 0 0 0	
2.466E-05	8.700E-03	ns	N323	0 0 0 0 0	

3749. C₁₇H₁₇Cl₂N

Sertraline

(1*S*-*cis*)-4-(3,4-dichlorophenyl)-1,2,3,4-tetrahydro-*N*-methyl-1-naphthalenamine

RN: 79617-96-2 MP (°C):
 MW: 306.24 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.27E-04	<1.00E-01	rt	B435	0 0 0 0 0	

3750. C₁₇H₁₇NO₂

Apomorphine

Apomorphin

RN: 58-00-4 MP (°C):
 MW: 267.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	1.069E-01	15	K059	2 2 2 0 0	
7.481E-02	2.000E+01	25	P312	0 0 0 0 0	

3751. C₁₇H₁₇NO₅

N-Benzylloxycarbonyl-L-tyrosine

Carbobenzoxytyrosine

RN: 1164-16-5 MP (°C):
 MW: 315.33 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.852E-03	1.530E+00	25.1	N026	0 0 0 0 0	

3752. C₁₇H₁₇N₅O₅9-[5'-(*O*-Benzoyl)-β-D-arabinofuranosyl]adenine ester

RN: 42782-57-0 MP (°C): 223.0
 MW: 371.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.154E-04	8.000E-02	ns	B134	0 1 1 1 0	

3753. C₁₇H₁₈ClNO₆

Griseofulvin-4'-oxime

Spiro[benzofuran-2(3H),1'-[2]cyclohexene]-3,4'-dione, 7-chloro-2',4,6-trimethoxy-6'-methyl-, 4'-oxime

RN: 13215-54-8 **MP (°C):**
MW: 367.79 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.589E-04	1.320E-01	37	F033	2 0 2 0 2	

3754. C₁₇H₁₈ClN₅O₆

Dis. A. 8

Ethanol, 2,2'--[[4-[(2-chloro-4,6-dinitrophenyl)azo]-3-methylphenyl]imino]bis-

RN: 65125-87-3 **MP (°C):**
MW: 423.82 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	2.119E-04	25	B333	0 0 0 0 0	

3755. C₁₇H₁₈Cl₂N₄O₄

Dis. A. 10

Ethanol, 2,2'-[4-(2,6-dichloro-4-nitrophenylazo)-*m*-tolylimino]di-

RN: 58528-60-2 **MP (°C):**
MW: 413.26 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-06	4.546E-04	25	B333	0 0 0 0 0	

3756. C₁₇H₁₈FN₃O₃

Ciprofloxacin

1-Cyclopropyl-6-fluoro-1,4-dihydro-4-oxo-7-(1-piperazinyl)-3-quinolinecarboxylic

Baycip

Velmonit

RN: 85721-33-1 **MP (°C):**
MW: 331.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.117E-04	3.700E-02	6	Y421	0 0 0 0 0	
1.630E-04	5.400E-02	22.5	B422	2 0 2 2 2	
2.595E-04	8.600E-02	25	Y421	0 0 0 0 0	
4.225E-04	1.400E-01	30	Y421	0 0 0 0 0	
5.131E-04	1.700E-01	40	Y421	0 0 0 0 0	
3.730E+00	1.236E+03	c	B443	0 0 0 0 0	

3757. C₁₇H₁₈N₂O₆

Nifedipine

3,5-Pyridinedicarboxylic acid

RN: 21829-25-4 MP (°C): 172–174

MW: 346.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.675E-05	5.800E-03	25	B387	0 0 0 0 0	
2.887E-05	1.000E-02	ns	K444	0 0 0 0 0	
1.738E-05	6.019E-03	ns	R427	0 0 0 0 0	

3758. C₁₇H₁₈N₄O₃S

4-Sulfanilamido-1-phenyl-2,3-dimethyl-5-pyrazolone

RN: 71119-16-9 MP (°C):

MW: 358.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.352E-04	1.560E-01	37	R045	1 2 1 1 2	

3759. C₁₇H₁₉CIN₂S

4-Chloropromazine

4-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide

RN: 13094-24-1 MP (°C):

MW: 318.87 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-05	3.508E-03	ns	G023	0 0 1 1 1	

3760. C₁₇H₁₉CIN₂S

3-Chloropromazine

3-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide

RN: 484-19-5 MP (°C):

MW: 318.87 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	3.189E-03	ns	G023	0 0 1 1 1	

3761. C₁₇H₁₉CIN₂S

1-Chloropromazine

1-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-propanamide

RN: 13100-13-5 MP (°C):

MW: 318.87 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-05	3.826E-03	0	G023	0 0 0 0 1	

3762. C₁₇H₁₉CIN₄O₄

C.I. Disperse red 5

Ethanol, 2,2'-[[4-[(2-chloro-4-nitrophenyl)azo]-3-methylphenyl]imino]bis-

RN: 3769-57-1 **MP (°C):** 192**MW:** 378.82 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-07	1.440E-04	25	B333	0 0 0 0 0	

3763. C₁₇H₁₉ClO₆

Griseofulvin-4'-ol

Spiro[benzofuran-2(3H),1'-[2]cyclohexen]-3-one, 7-chloro-4'-hydroxy-2',4,6-trimethoxy-6'-methyl-

RN: 13215-53-7 **MP (°C):****MW:** 354.79 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.129E-04	2.529E-01	37	F033	2 0 2 0 2	average of 2

3764. C₁₇H₁₉NO₃

Piperine

Piperidine, 1-[5-(1,3-benzodioxol-5-yl)-1-oxo-2,4-pentadienyl]-, (E,E)-N-[(E,E)-Piperoyl]piperidine

RN: 94-62-2 **MP (°C):** 130.0**MW:** 285.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	3.995E-02	15	K059	2 2 2 0 1	
1.402E-04	4.000E-02	18	F300	1 0 0 0 0	
3.504E-04	9.999E-02	rt	D021	0 0 1 1 0	

3765. C₁₇H₁₉NO₃1-Methyl-1-nitro-2-(*p*-methylphenyl)-2-*p*-ethoxyphenyl)ethane**RN:** 53982-07-3 **MP (°C):****MW:** 285.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.060E-06	2.300E-03	rt	C122	0 0 0 0 0	

3766. C₁₇H₁₉NO₃

Hydromorphone

Dilauidid

PMS-Hydromorphone

Dihydromorphinone

RN: 466-99-9

MP (°C):

MW: 285.35

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.767E-03	1.931E+00	25	R338	0 0 0 0 0	

3767. C₁₇H₁₉NO₃

Morphine

Morphin

7,8-Didehydro-4,5-epoxy-17-methylmorphinan-3,6-diol

RN: 57-27-2 MP (°C): 254dec

MW: 285.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	1.427E-01	15	K059	2 2 2 0 0	
5.222E-04	1.490E-01	20	B061	1 0 1 1 2	
5.257E-04	1.500E-01	20	F300	1 0 0 0 0	
1.209E-03	3.450E-01	25	R338	0 0 0 0 0	
7.200E-04	2.054E-01	30	L068	1 0 0 1 0	EFG
1.000E-03	2.853E-01	30	L069	1 0 1 1 0	EFG
8.761E-04	2.500E-01	35	R418	0 0 0 0 0	Intrinsic
1.051E-03	2.999E-01	rt	D021	0 0 1 1 0	

3768. C₁₇H₁₉NO₃H₂O

Morphine (monohydrate)

Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl-(5α,6α)-, monohydrate

RN: 6009-81-0 MP (°C): 254dec

MW: 303.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.328E-04	2.830E-01	c	D004	0 0 0 0 0	
3.064E-03	9.294E-01	h	D004	0 0 0 0 0	

3769. C₁₇H₁₉NO₄1-Methyl-1-nitro-2,2-bis(*p*-methoxylphenyl)ethane

RN: 34197-26-7 MP (°C):

MW: 301.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.854E-05	8.600E-03	rt	C122	0 0 0 0 0	

3770. C₁₇H₁₉N₃

Antazoline

Albalon-A

RN: 91-75-8

MP (°C): 120

MW: 265.36

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-03	6.634E-01	30	L068	1 0 0 1 0	EFG
1.900E-02	5.042E+00	37.5	L034	2 2 0 1 2	pH 7.4

3771. C₁₇H₁₉N₅O₆

Dis. A. 1

Ethanol, 2,2'-[4-(2,4-dinitrophenylazo)-*m*-tolylimino]di-

Disperse violet 4K

Terasil violet P 4RT

RN: 41541-13-3 MP (°C): 190

MW: 389.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-07	2.726E-04	25	B333	0 0 0 0 0	

3772. C₁₇H₂₀CIN₅O₂

1H-Purine-2,6-dione, 8-(2-amino-4-chlorophenyl)-3,7-dihydro-1,3-dipropyl-1,3-Dipropyl-8-(2-amino-4-chlorophenyl)xanthine

PACPX

RN: 85872-51-1 MP (°C):

MW: 361.83 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.76E-07	<1.00E-04	ns	H316	0 0 0 0 0	pH 7.4
1.105E-06	4.000E-04	ns	H316	0 0 0 0 0	0.1N HCL

3773. C₁₇H₂₀N₂O

Michler's ketone

Tetramethyldiaminobenzophenone

bis[4-(Dimethylamino)phenyl]-methanone

p,p'-bis(*N,N*-Dimethylamino)benzophenone4,4-[*bis*(Dimethylamino)benzophenone

RN: 90-94-8 MP (°C): 172.0

MW: 268.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-03	3.998E-01	rt	D021	0 0 1 1 0	

3774. C₁₇H₂₀N₂O₂

Tropicamide

RN: 1508-75-4

MP (°C):

MW: 284.36

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.032E-04	2.000E-01	25	C414	1 0 1 1 0	EFG

3775. C₁₇H₂₀N₂S

Promethazine

10-(2-Dimethylaminopropyl)phenothiazine

10-(2-Dimethylamino-2-methylethyl)phenothiazine

Fenergan

Protazine

Thiergan

RN: 60-87-7

MP (°C): 60

MW: 284.43

BP (°C): 191

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-06	3.839E-04	22.5	B440	0 0 0 0 0	
5.500E-05	1.564E-02	24	G023	2 0 1 1 1	
4.390E+00	1.249E+03	c	B443	0 0 0 0 0	

3776. C₁₇H₂₀N₂S

Promazine

Primazine

Sparine

Prozine

RN: 58-40-2

MP (°C): 32

MW: 284.43

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.422E-02	24	G023	2 0 1 1 1	
5.000E-05	1.422E-02	ns	G023	0 0 0 0 1	

3777. C₁₇H₂₀N₄O₄

C.I. Disperse red 17

Ethanol, 2,2'-[{[3-methyl-4-[(4-nitrophenyl)azo]phenyl]imino]bis-

RN: 3179-89-3 MP (°C): 160

MW: 344.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-06	6.199E-04	25	B333	0 0 0 0 0	

3778. C₁₇H₂₀N₄O₅

Dis. A. 13

4-Nitro-2-methoxy-4'-di(β-hydroxyethyl)-aminoazobenzene

Ethanol, 2,2'--[[4-[(2-methoxy-4-nitrophenyl)azo]phenyl]imino]bis

Ethanol, 2,2'-[*p*-(2-methoxy-4-nitrophenylazo)phenylimino]di-**RN:** 41541-14-4 **MP (°C):****MW:** 360.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	7.207E-03	25	B333	0 0 0 0 0	
6.826E-04	2.460E-01	100	P313	0 0 0 0 0	

3779. C₁₇H₂₀N₄O₅S

Benzenesulfonic acid, 4-(2,3,6,7-tetrahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)-

RN: 89073-57-4 **MP (°C):****MW:** 392.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.313E-03	1.300E+00	ns	H316	0 0 0 0 0	0.1N HCL
>6.12E-02	>2.40E+01	ns	H316	0 0 0 0 0	pH 7.4

3780. C₁₇H₂₀N₄O₆

Riboflavin

Riboflavin

Robiflavin

7,8-Dimethyl-10-ribitylisalloxazine

Zinvit-G

E-101

RN: 83-88-5 **MP (°C):** 290**MW:** 376.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.657E-04	9.999E-02	20	A022	1 0 0 0 0	
2.250E-04	8.468E-02	25	A079	1 0 1 1 2	
2.657E-04	9.999E-02	25	D041	1 0 0 0 0	
1.754E-04	6.600E-02	25	D315	0 0 0 0 0	
2.192E-04	8.250E-02	30	C409	2 0 1 2 2	
3.959E-04	1.490E-01	37	E018	1 0 2 1 2	
2.089E-04	7.864E-02	ns	R427	0 0 0 0 0	

3781. C₁₇H₂₀O₆

Mycophenolic acid

6-(1,3-Dihydro-7-hydroxy-5-methoxy-4-methyl-1-oxoisobenzofuran-6-yl)-4-methyl-4-hexanoic acid

RN: 24280-93-1 MP (°C):

MW: 320.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.058E-05	1.300E-02	25	L333	1 1 1 1 0	

3782. C₁₇H₂₁NO₂

Napropamide

N,N-Diethyl-2-(1-naphthoxy)propanamide

Devrinol 50W

Devrinol

Devrinol 10G

Devrinol 2E

RN: 15299-99-7 MP (°C): 75.1

MW: 271.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.690E-04	7.300E-02	20	M161	1 0 0 0 1	

3783. C₁₇H₂₁NO₃

Etodolac

(+-)-1,8-Diethyl-1,3,4,9-tetrahydropyrano-(3,4-b)indole-1-acetic acid

Lodine

RN: 41340-25-4 MP (°C):

MW: 287.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.392E-04	4.000E-02	37	Y421	0 0 0 0 0	

3784. C₁₇H₂₁NO₄

Scopolamine

Scopolamin

Hyoscine

Murocoll

Plexonal

Transderm-SCOP

RN: 51-34-3 MP (°C): 59

MW: 303.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.132E-01	9.500E+01	15	F300	1 0 0 0 1	
3.296E-01	1.000E+02	ns	C109	0 0 0 0 1	

3785. C₁₇H₂₁NO₄

Cocaine

L-Cocaine

L-Cocain

RN: 50-36-2**MP (°C):** 98**MW:** 303.36**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-03	1.213E+00	15	K059	2 2 2 0 0	
5.934E-03	1.800E+00	22	F300	1 0 0 0 1	
5.485E-03	1.664E+00	25	D004	0 0 0 0 0	
5.266E-03	1.597E+00	25	D041	1 0 0 0 1	
1.248E-02	3.786E+00	80	D041	1 0 0 0 1	

3786. C₁₇H₂₁N₃O₂

Dis. A. 2

Ethanol, 2,2'-[[3-methyl-4-(phenylazo)phenyl]imino]bis-4-[bis(2-Hydroxyethyl)amino]-2-methylazobenzene

RN: 3771-38-8**MP (°C):** 111**MW:** 299.38**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.600E-05	2.275E-02	25	B333	0 0 0 0 0	

3787. C₁₇H₂₁N₅O₂

1H-Purine-2,6-dione, 8-(2-aminophenyl)-3,7-dihydro-1,3-dipropyl-

RN: 96445-34-0**MP (°C):** 276dec**MW:** 327.39**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.05E-06	<1.00E-03	ns	H316	0 0 0 0 0	pH 7.4
1.222E-05	4.000E-03	ns	H316	0 0 0 0 0	0.1N HCL

3788. C₁₇H₂₁N₅O₁₀

9-(1,3-Dihemisuccinate-2-propoxymethyl)guanine

RN: 88110-76-3**MP (°C):** 167**MW:** 455.38**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.039E-01	4.730E+01	25	B360	0 0 0 0 0	

3789. C₁₇H₂₂I₃N₃O₈

1,3-Benzenedicarboxamide, *N,N'*-bis(2,3-dihydroxypropyl)-5*S*RS-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS*^{*},*RS*^{*})]-

RN: 60166-94-1 **MP (°C):**
MW: 777.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3790. C₁₇H₂₂I₃N₃O₈

1,3-Benzenedicarboxamide, *N,N'*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS*^{*},*RS*^{*})]-

RN: 77942-93-9 **MP (°C):**
MW: 777.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.480E-01	1.150E+02	25	P091	0 0 0 0 0	

3791. C₁₇H₂₂I₃N₃O₈

1,3-Benzenedicarboxamide, *N*-(2,3-dihydroxypropyl)-*N'*-[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-

RN: 77868-45-2 **MP (°C):**
MW: 777.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3792. C₁₇H₂₂I₃N₃O₈

1,3-Benzenedicarboxamide, *N,N'*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*S*-(*S*^{*},*S*^{*})]-

RN: **MP (°C):**
MW: 777.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3793. C₁₇H₂₂I₃N₃O₈

DL-Iopamidol

1,3-Benzenedicarboxamide, *N,N'*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*S*)-

L-Iopamidol

1,3-Benzenedicarboxamide, *N,N'*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*S**,*S**)]**RN:** 60166-93-0 **MP (°C):****MW:** 777.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.096E-01	4.737E+02	20	F178	1 0 0 0 1	EFG
1.580E-01	1.228E+02	20	F178	1 0 0 0 1	EFG
6.096E-01	4.737E+02	25	P091	0 0 0 0 0	
1.580E-01	1.228E+02	25	P091	0 0 0 0 0	
5.798E-01	4.505E+02	40	F178	1 0 0 0 1	EFG
1.963E-01	1.525E+02	40	F178	1 0 0 0 1	EFG
5.679E-01	4.413E+02	60	F178	1 0 0 0 1	EFG
3.120E-01	2.424E+02	60	F178	1 0 0 0 1	EFG
6.235E-01	4.845E+02	80	F178	1 0 0 0 1	EFG
5.209E-01	4.048E+02	80	F178	1 0 0 0 1	EFG
6.911E-01	5.370E+02	100	F178	1 0 0 0 1	EFG
7.098E-01	5.516E+02	100	F178	1 0 0 0 1	EFG

3794. C₁₇H₂₂I₃N₃O₈1,3-Benzenedicarboxamide, *N,N'*-bis(2,3-dihydroxypropyl)-5*RS*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-[*RS*-(*RS**,*S**)]-**RN:** **MP (°C):****MW:** 777.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3795. C₁₇H₂₂I₃N₃O₈1,3-Benzenedicarboxamide, *N,N'*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-, (*RS*)-**RN:** 60208-45-9 **MP (°C):****MW:** 777.09 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.775E-01	1.379E+02	25	P091	0 0 0 0 0	

3796. C₁₇H₂₂I₃N₃O₈

1,3-Benzeneddicarboxamide, *N,N'*-bis(2,3-dihydroxypropyl)-5*S*-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triiodo-(*RS,S*)-

RN: MP (°C):
MW: 777.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.379E-01	1.071E+02	25	P091	0 0 0 0 0	

3797. C₁₇H₂₂I₃N₃O₉

1,3-Benzeneddicarboxamide, 5-[(2,3-dihydroxy-1-oxopropyl)amino]-*N,N'*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 69698-47-1 MP (°C):
MW: 793.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.573E-02	5.213E+01	25	P091	0 0 0 0 0	

3798. C₁₇H₂₂I₃N₃O₉

1,3-Benzeneddicarboxamide, 5-[(2,3-dihydroxy-1-oxobutyl)amino]-*N,N'*-bis[2-hydroxy-1-(hydroxymethyl)ethyl]-2,4,6-triiodo-

RN: 129968-26-9 MP (°C):
MW: 793.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.430E-02	4.306E+01	25	P091	0 0 0 0 0	

3799. C₁₇H₂₂N₄O₃S

2-(*N*4-Acetylulfanilylamo)-4-*n*-amylpyrimidine

RN: MP (°C):
MW: 362.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.214E-05	4.400E-03	37	R076	1 2 0 0 1	

3800. C₁₇H₂₂N₄O₇.0.75H₂O

2'-(2-Methyl-3-one-pentanyl)-6-methoxypurine arabinoside (0.75 hydrate)

RN: 145913-50-4 MP (°C): 55–60
MW: 407.90 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.770E-02	3.577E+01	37	C348	0 0 0 0 0	pH 7.00

3801. C₁₇H₂₃NO*N,N*-Octamethylenecinnamamide

Octahydro-1-(1-oxo-3-phenyl-2-propenyl)1H-azonine

RN: 59832-07-4 MP (°C):

MW: 257.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.460E-04	6.332E-02	ns	H350	0 0 0 0 0	

3802. C₁₇H₂₃NO*N*-Cyclooctylcinnamamide2-Propenamide, *N*-cyclooctyl-3-phenyl-

RN: 59832-00-7 MP (°C):

MW: 257.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.660E-06	6.846E-04	ns	H350	0 0 0 0 0	

3803. C₁₇H₂₃NO₃

Hyoscyamine

Hyoscyamin

Benzeneacetic acid, α-(hydroxymethyl)-, 8-methyl-8-azabicyclo[3.2.1]oct-3-yl ester, [3(S)-*endo*]-Daturine

Duboisine

L-Hyoscyamine

RN: 101-31-5 MP (°C): 108.5

MW: 289.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.244E-02	3.600E+00	20	F300	1 0 0 0 2	
1.225E-02	3.546E+00	c	D004	0 0 0 0 0	

3804. C₁₇H₂₃NO₃

Atropine

Atropin

8-Methyl-8-azabicyclo[3.2.1]octan-3-yl 3-hydroxy-2-phenylpropionate

Neo-diophen

Minims

RN: 51-55-8 MP (°C): 115

MW: 289.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-03	1.592E+00	15	K059	2 2 2 0 1	
5.529E-03	1.600E+00	18	F300	1 0 0 0 1	

(continued)

3804. C₁₇H₂₃NO₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.898E-03	1.996E+00	20	D041	1 0 0 0 0	
1.032E-02	2.987E+00	20	K052	1 1 1 1 2	
1.610E+00	4.659E+02	25	B443	0 0 0 0 0	
1.148E-02	3.322E+00	25	D004	0 0 0 0 0	
7.586E-03	2.195E+00	rt	D021	0 0 1 1 1	

3805. C₁₇H₂₃NO₅

Benzoic acid, 2-(acetoxy)-, 2-[bis(1-methylethyl)amino]-2-oxoethyl ester

RN: 116482-76-9 MP (°C): 108.9

MW: 321.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.601E-04	1.800E-01	21	N335	0 0 0 0 0	

3806. C₁₇H₂₃NO₅

Benzoic acid, 2-(acetoxy)-, 2-(dipropylamino)-2-oxoethyl ester

RN: 116482-75-8 MP (°C): 50.5

MW: 321.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-03	7.200E-01	21	N335	0 0 0 0 0	

3807. C₁₇H₂₃N₃O

Aeo-antergan

1,2-Ethanediamine, N-[(4-methoxyphenyl)methyl]-N',N'-dimethyl-N-2-pyridinyl-

Dorantamin

Anthisan

Dipane

Copsamine

RN: 91-84-9 MP (°C):

MW: 285.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-02	3.425E+00	37.5	L034	2 2 0 1 2	pH 7.4

3808. C₁₇H₂₃N₃O₂

2-Methoxy-N-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide
N-[2-(Diethylamino)ethyl]-2-methoxyquinoline-4-carboxamide

RN: 2716-98-5 **MP (°C):**
MW: 301.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-03	9.042E-01	ns	B018	0 0 0 0 1	
3.000E-03	9.042E-01	ns	M066	0 0 0 0 0	

3809. C₁₇H₂₄N₄O₅

1,5-Dipivaloyloxyethyl allopurinol
RN: 98827-16-8 **MP (°C):** 136–137
MW: 364.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.488E-05	2.000E-02	22	B322	0 0 0 0 0	
5.495E-05	2.003E-02	ns	R427	0 0 0 0 0	

3810. C₁₇H₂₄N₄O₅

2,5-Dipivaloyloxyethyl allopurinol
RN: 98827-17-9 **MP (°C):** 145–146
MW: 364.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.235E-04	4.500E-02	22	B322	0 0 0 0 0	

3811. C₁₇H₂₄N₄O₆

2'-Hexanyl-6-methoxypurine arabinoside
RN: 145913-39-9 **MP (°C):**
MW: 380.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.890E-02	7.190E+00	37	C348	0 0 0 0 0	pH 7.00

3812. C₁₇H₂₅NO

N-Octylcinnamamide
 2-Propenamide, *N*-octyl-3-phenyl-
RN: 55030-48-3 **MP (°C):**
MW: 259.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.390E-06	3.606E-04	ns	H350	0 0 0 0 0	

3813. C₁₇H₂₅NO₃

Acetamide, 2-(benzoyloxy)-N,N-bis(2-methylpropyl)-

RN: 115193-33-4 **MP (°C):** 44.5**MW:** 291.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-04	8.000E-02	22	N317	1 1 2 1 2	

3814. C₁₇H₂₅NO₃

Acetamide, 2-(benzoyloxy)-N,N-acetamide, 2-(benzoyloxy)-N,N-dibutyl-

RN: 106231-57-6 **MP (°C):** 25**MW:** 291.39 **BP (°C):** 428.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.745E-04	8.000E-02	22	B427	1 0 0 1 1	in 0.01M HCl
2.745E-04	8.000E-02	22	N317	1 1 2 1 2	

3815. C₁₇H₂₅NO₄

Octyl acetaminophen

Carbonic acid, octyl ester, ester with 4'-hydroxyacetanilide

Acetanilide, 4'-hydroxy-, octyl carbonate (ester)

RN: 19872-70-9 **MP (°C):** 82.5–83**MW:** 307.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-05	4.400E-03	37	D029	0 0 0 0 0	

3816. C₁₇H₂₅N₅O₆

9-(1,3-Dibutyrate-2-propoxymethyl)guanine

RN: 88110-71-8 **MP (°C):** 200**MW:** 395.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.541E-04	1.400E-01	25	B360	0 0 0 0 0	

3817. C₁₇H₂₆ClNO₂

Butachlor

N-(Butoxymethyl)-2-chloro-N-(2,6-diethylphenyl)acetamide

N-(Butoxymethyl)-2-chloro-2',6'-diethylacetanilide

Machete

Butanex

Hiltachlor

RN: 23184-66-9 **MP (°C):** <-5**MW:** 311.86 **BP (°C):** 196

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.413E-05	2.000E-02	20	M161	1 0 0 0 1	
6.412E-05	2.000E-02	ns	S460	0 0 0 0 0	
7.055E-05	2.200E-02	ns	Y414	0 0 0 0 0	
7.055E-02	2.200E+01	ns	Y414	0 0 0 0 0	

3818. C₁₇H₂₆O₃Decyl-*p*-hydroxybenzoateDecyl *p*-hydroxybenzoate*n*-Decyl *p*-hydroxybenzoate**RN:** 69679-30-7 **MP (°C):** 58**MW:** 278.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-05	8.909E-03	15	B355	0 0 0 0 0	
3.710E-05	1.033E-02	20	B355	0 0 0 0 0	
8.800E-05	2.450E-02	25	B355	0 0 0 0 0	
1.303E-03	3.629E-01	25	D081	1 2 2 1 2	<i>sic</i>
7.943E-05	2.211E-02	25	F322	2 0 1 1 0	EFG

3819. C₁₇H₂₇NO₂

Terbutol

2,6-Di-*tert*-butyl-*p*-tolyl methylcarbamate**RN:** 1918-11-2 **MP (°C):** 185**MW:** 277.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.343E-05	6.500E-03	25	B200	1 0 0 0 0	
2.523E-05	7.000E-03	ns	H042	0 0 0 0 0	

3820. C₁₇H₂₇NO₂

Venlafaxine

RN: 93413-69-5 **MP (°C):**
MW: 277.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.60E-04	<1.00E-01	rt	B435	0 0 0 0 0	

3821. C₁₇H₂₇NO₃

Pramoxine

Pramocaine

RN: 140-65-8 **MP (°C):**
MW: 293.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.218E-05	3.574E-03	22.5	B440	0 0 0 0 0	

3822. C₁₇H₂₇NO₃

Stadacain

4-Butoxybenzoic acid 2-(diethyl-amino)ethyl ester

RN: 2350-32-5 **MP (°C):** 146
MW: 293.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	3.814E-02	ns	M066	0 0 0 0 1	

3823. C₁₇H₂₇NO₄

Nadolol

Corgard

Nadolol

RN: 42200-33-9 **MP (°C):**
MW: 309.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.683E-02	8.300E+00	25	A412	1 0 2 2 1	int

3824. C₁₇H₂₈

4-Phenylundecane

RN: **MP (°C):**
MW: 232.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-09	2.092E-06	25	S377	0 0 0 0 0	

3825. C₁₇H₂₈

6-Phenylundecane

RN:**MW:** 232.41**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-08	2.557E-06	25	S377	0 0 0 0 0	

3826. C₁₇H₂₈

3-Phenylundecane

RN:**MW:** 232.41**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-08	2.789E-06	25	S377	0 0 0 0 0	

3827. C₁₇H₂₈

2-Phenylundecane

RN:**MW:** 232.41**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-09	1.859E-06	25	S377	0 0 0 0 0	

3828. C₁₇H₂₈

5-Phenylundecane

RN:**MW:** 232.41**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-08	2.324E-06	25	S377	0 0 0 0 0	

3829. C₁₇H₂₈N₂O₂

4-Butylaminobenzoic acid 2-(diethyl-amino)ethyl ester

RN: 3772-42-7**MP (°C):****MW:** 292.42**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-04	1.199E-01	ns	M066	0 0 0 0 1	

3830. C₁₇H₂₈N₂O₂

Endomid

N,N,N',N'-Tetraethyl-bicyclo(2.2.1)hept-5-ene-2,3-dicarboxamide

RN: 4582-18-7 **MP (°C):****MW:** 292.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.916E-02	1.730E+01	20	K050	1 1 1 1 2	

3831. C₁₇H₂₈O₂

4-Nonylphenol monoethoxylate

Ethanol, 2-(4-nonylphenoxy)-

RN: 104-35-8 **MP (°C):****MW:** 264.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.048E-05	2.770E-03	2	A335	0 0 0 0 0	
1.050E-05	2.776E-03	2	A335	0 0 0 0 0	
1.063E-05	2.810E-03	10	A335	0 0 0 0 0	
1.060E-05	2.803E-03	10	A335	0 0 0 0 0	
1.074E-05	2.840E-03	14	A335	0 0 0 0 0	
1.080E-05	2.856E-03	14	A335	0 0 0 0 0	
1.140E-05	3.014E-03	20.5	A335	0 0 0 0 0	
1.142E-05	3.020E-03	20.5	A335	0 0 0 0 0	
1.280E-05	3.384E-03	25	A335	0 0 0 0 0	
1.275E-05	3.370E-03	25	A335	0 0 0 0 0	

3832. C₁₇H₃₄O₂

Margaric acid

Heptadecanoic acid

RN: 506-12-7 **MP (°C):****MW:** 270.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.035E-05	2.800E-03	0	B136	1 0 2 1 1	
1.553E-05	4.200E-03	20	B136	1 0 2 1 1	
1.553E-05	4.200E-03	20.0	R001	1 1 1 1 1	
1.997E-05	5.400E-03	30	B136	1 0 2 1 1	
2.034E-05	5.500E-03	30.0	R001	1 1 1 1 1	
2.551E-05	6.900E-03	45	B136	1 0 2 1 1	
2.551E-05	6.900E-03	45.0	R001	1 1 1 1 1	
2.995E-05	8.100E-03	60	B136	1 0 2 1 1	
2.995E-05	8.100E-03	60.0	R001	1 1 1 1 1	
1.035E-05	2.800E-03	.0	R001	1 1 1 1 1	

3833. C₁₇H₃₆N₂Ge

Spirogermanium

2-[3-(Dimethylamino)propyl]-8,8-diethyl-2-aza-8-germaspiro[4.5]decane

RN: 41992-23-8 MP (°C):

MW: 341.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.463E-05	8.400E-03	22	M456	0 0 0 0 0	pH 12.5

3834. C₁₇H₃₆O

Heptadecanol

1-Heptadecanol

RN: 1454-85-9 MP (°C): 58

MW: 256.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<=1E-7	<=2.56E-5	25	R002	0 0 0 0 0	

3835. C₁₈H₁₀Cl₄2,4,4",6-Tetrachloro-*p*-terphenyl

2,4,4",6-Tetrachloro-1,1':4',1"-terphenyl

RN: 61576-97-4 MP (°C):

MW: 368.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.606E-10	5.910E-08	4	D351	1 2 1 1 2	
4.728E-10	1.740E-07	25	D351	1 2 1 1 2	
1.106E-09	4.069E-07	40	D351	1 2 1 1 2	

3836. C₁₈H₁₀I₆N₂O₇

Ioglycamic acid

N,N'-bis(3-Carboxy-2,4,6-triodophenyl)-diglycolamide

BE 419

RN: 2618-25-9 MP (°C):

MW: 1127.72 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.773E-04	2.000E-01	ns	H055	0 0 0 0 0	

3837. C₁₈H₁₀N₂O₂S

Disperse brightener

2,2'-(2,5-Thiophenediyi)bisbenzoxazole

Unitex OB

Uvitex EBF

RN: 2866-43-5 **MP (°C):** 219**MW:** 318.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-08	9.551E-06	25	B333	0 0 0 0 0	

3838. C₁₈H₁₁Cl₃2,4",5-Trichloro-*p*-terphenyl

2,4",5-Trichloro-1,1':4',1"-terphenyl

RN: 61576-93-0 **MP (°C):****MW:** 333.65 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.028E-10	1.010E-07	4	D351	1 2 1 1 2	
1.233E-09	4.115E-07	25	D351	1 2 1 1 2	
2.567E-09	8.564E-07	39	D351	1 2 1 1 2	

3839. C₁₈H₁₁NO₃

Samaron yellow

Supra light yellow GGL(IG)

RN: 1326-08-5 **MP (°C):****MW:** 289.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-06	1.157E-03	98.59	M180	0 0 2 2 0	EFG
8.000E-06	2.314E-03	111.46	M180	0 0 2 2 0	EFG
1.000E-05	2.893E-03	112.94	M180	0 0 2 2 0	EFG
1.100E-05	3.182E-03	119.00	M180	0 0 2 2 0	EFG
1.300E-05	3.761E-03	125.25	M180	0 0 2 2 0	EFG
1.400E-05	4.050E-03	128.45	M180	0 0 2 2 0	EFG
2.200E-05	6.364E-03	152.37	M180	0 0 2 2 0	EFG

3840. C₁₈H₁₁NO₃

Disperse yellow 54

C.I. Disperse yellow 54

RN: 7576-65-0 **MP (°C):****MW:** 289.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-07	2.893E-05	25	B333	0 0 0 0 0	
2.400E-07	6.943E-05	60.0	D093	1 2 1 2 0	EFG (continued)

3840. C₁₈H₁₁NO₃ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-07	1.880E-04	71.8	D093	1 2 1 2 0	EFG
1.600E-06	4.629E-04	84.1	D093	1 2 1 2 0	EFG
4.000E-06	1.157E-03	97.4	D093	1 2 1 2 0	EFG

3841. C₁₈H₁₂

Tetracene

Naphthacene

2,3-Benzanthracene

RN: 92-24-0 MP (°C): 341

MW: 228.30 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-08	3.607E-06	20	E009	1 0 0 1 2	
6.600E-09	1.507E-06	25	K001	2 2 2 2 1	
2.497E-09	5.700E-07	25	M064	1 1 2 2 1	
2.500E-09	5.707E-07	25	M342	1 0 1 1 1	
4.380E-09	1.000E-06	27	D003	1 0 0 1 1	
2.497E-09	5.700E-07	ns	M344	0 0 0 0 2	
2.754E-09	6.288E-07	ns	R424	0 0 0 0 0	

3842. C₁₈H₁₂

Triphenylene

9,10-Benzphenanthrene

Isochrysene

RN: 217-59-4 MP (°C): 199

MW: 228.30 BP (°C): 425

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-08	2.694E-06	8	M082	1 1 1 2 2	
1.180E-08	2.694E-06	8	M151	2 1 2 2 2	
1.311E-08	2.992E-06	8.04	M183	1 2 1 1 2	
1.330E-08	3.036E-06	12.00	M082	1 1 1 2 2	
1.330E-08	3.036E-06	12.00	M151	2 1 2 2 2	
1.328E-08	3.033E-06	12.04	M183	1 2 1 1 2	
1.490E-08	3.402E-06	14.80	M082	1 1 1 2 2	
1.490E-08	3.402E-06	14.80	M151	2 1 2 2 2	
2.500E-07	5.707E-05	20	E009	1 0 0 1 1	
2.140E-08	4.886E-06	20.50	M082	1 1 1 2 2	
2.140E-08	4.886E-06	20.50	M151	2 1 2 2 2	
2.144E-08	4.894E-06	20.54	M183	1 2 1 1 2	
1.800E-07	4.109E-05	25	A325	2 1 2 2 1	
1.880E-07	4.292E-05	25	K001	1 0 2 1 2	
1.884E-07	4.300E-05	25	M064	1 1 2 2 1	
2.891E-08	6.600E-06	25.00	M151	2 1 1 2 1	
1.665E-07	3.800E-05	27	D003	1 0 0 1 1	
3.350E-08	7.648E-06	27.30	M082	1 1 1 2 2	

(continued)

3842. C₁₈H₁₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.350E-08	7.648E-06	27.30	M151	2 1 2 2 2	
3.354E-08	7.657E-06	27.34	M183	1 2 1 1 2	
3.550E-08	8.105E-06	28.20	M082	1 1 1 2 2	
3.550E-08	8.105E-06	28.20	M151	2 1 2 2 2	
3.556E-08	8.117E-06	28.24	M183	1 2 1 1 2	
1.486E-08	3.393E-06	114.84	M183	1 2 1 1 2	
1.884E-07	4.300E-05	ns	M344	0 0 0 0 2	

3843. C₁₈H₁₂

1,2-Benzanthracene

Benzanthracene

1,2-Benzoanthracene

RN: 56-55-3

MP (°C): 155

MW: 228.30

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.310E-08	2.991E-06	6.90	M082	1 1 1 2 2	
1.310E-08	2.991E-06	6.90	M151	2 1 2 2 2	
1.311E-08	2.992E-06	6.94	M183	1 2 1 1 2	
1.660E-08	3.790E-06	10.70	M082	1 1 1 2 2	
1.660E-08	3.790E-06	10.70	M151	2 1 2 2 2	
1.657E-08	3.783E-06	11.14	M183	1 2 1 1 2	
2.100E-08	4.794E-06	14.24	M183	1 2 1 1 2	
2.100E-08	4.794E-06	14.30	M082	1 1 1 2 2	
2.100E-08	4.794E-06	14.30	M151	2 1 2 2 2	
1.583E-08	3.613E-06	14.34	M183	1 2 1 1 2	
2.365E-08	5.400E-06	15	B385	0 0 0 0 0	
2.446E-08	5.584E-06	18.14	M183	1 2 1 1 2	
2.770E-08	6.324E-06	19.30	M082	1 1 1 2 2	
2.770E-08	6.324E-06	19.30	M151	2 1 2 2 2	
2.775E-08	6.335E-06	19.34	M183	1 2 1 1 2	
3.670E-08	8.378E-06	23.10	M082	1 1 1 2 2	
3.670E-08	8.378E-06	23.10	M151	2 1 2 2 2	
3.669E-08	8.377E-06	23.14	M183	1 2 1 1 2	
3.507E-08	8.007E-06	23.64	M183	1 2 1 1 2	
1.927E-07	4.400E-05	24	H116	2 1 0 0 1	
4.117E-08	9.400E-06	25	B319	2 0 1 2 1	
4.056E-08	9.260E-06	25	B385	0 0 0 0 0	
5.694E-08	1.300E-05	25	D406	1 2 2 2 2	
4.310E-08	9.840E-06	25	K001	2 2 2 2 2	
3.900E-09	8.904E-07	25	K123	1 0 2 2 1	sic
2.497E-08	5.700E-06	25	L332	1 1 1 1 2	
6.132E-08	1.400E-05	25	M064	1 1 2 2 1	
4.117E-08	9.400E-06	25	M071	2 2 2 2 2	
6.130E-08	1.399E-05	25	M342	1 0 1 1 2	
4.117E-08	9.400E-06	25.00	M151	2 1 1 2 1	
3.774E-08	8.617E-06	25.04	M183	1 2 1 1 2	
4.818E-08	1.100E-05	27	D003	1 0 0 1 1	

(continued)

3843. C₁₈H₁₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.344E-08	1.220E-05	29	M071	2 2 2 2 2	
5.344E-08	1.220E-05	29.00	M151	2 1 1 2 2	
5.436E-08	1.241E-05	29.54	M183	1 2 1 1 2	
5.580E-08	1.274E-05	29.70	M082	1 1 1 2 2	
5.580E-08	1.274E-05	29.70	M151	2 1 2 2 2	
5.567E-08	1.271E-05	29.74	M183	1 2 1 1 2	
7.635E-08	1.743E-05	35	B385	0 0 0 0 0	
6.132E-08	1.400E-05	ns	M344	0 0 0 0 2	

3844. C₁₈H₁₂

Chrysene

1,2-Benzphenanthrene

RN: 218-01-9 **MP (°C):** 254
MW: 228.30 **BP (°C):** 448

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-09	7.077E-07	6.50	M082	1 1 1 2 2	
3.100E-09	7.077E-07	6.50	M151	2 1 2 2 2	
3.500E-09	7.990E-07	11.00	M082	1 1 1 2 2	
3.500E-09	7.990E-07	11.00	M151	2 1 2 2 2	
6.130E-09	1.399E-06	20.40	M082	1 1 1 2 2	
6.130E-09	1.399E-06	20.40	M151	2 1 2 2 2	
6.139E-09	1.401E-06	20.44	M183	1 2 1 1 2	
9.199E-09	2.100E-06	23	P339	0 0 0 0 0	
7.446E-08	1.700E-05	24	H116	2 1 0 0 1	
7.360E-09	1.680E-06	24.00	M082	1 1 1 2 2	
7.360E-09	1.680E-06	24.00	M151	2 1 2 2 2	
7.367E-09	1.682E-06	24.04	M183	1 2 1 1 2	
4.818E-09	1.100E-06	25	B319	2 0 1 2 1	average of 2
6.570E-09	1.500E-06	25	D406	1 2 2 2 2	
2.760E-08	6.301E-06	25	K001	2 2 2 2 2	
2.628E-08	6.000E-06	25	L332	1 1 1 1 2	
8.761E-09	2.000E-06	25	M064	1 1 2 2 1	
7.884E-09	1.800E-06	25	M071	2 2 2 2 2	
8.760E-09	2.000E-06	25	M342	1 0 1 1 2	
7.884E-09	1.800E-06	25.00	M151	2 1 1 2 1	
8.280E-09	1.890E-06	25.30	M082	1 1 1 2 2	
8.280E-09	1.890E-06	25.30	M151	2 1 2 2 2	
8.283E-09	1.891E-06	25.34	M183	1 2 1 1 2	
6.570E-09	1.500E-06	27	D003	1 0 0 1 1	
9.680E-09	2.210E-06	28.70	M082	1 1 1 2 2	
9.680E-09	2.210E-06	28.70	M151	2 1 2 2 2	
9.689E-09	2.212E-06	28.74	M183	1 2 1 1 2	
9.637E-09	2.200E-06	29	M071	2 2 2 2 2	
9.637E-09	2.200E-06	29.00	M151	2 1 1 2 1	
8.761E-09	2.000E-06	ns	M344	0 0 0 0 2	
8.710E-09	1.988E-06	ns	R424	0 0 0 0 0	
3.400E-06	7.762E-04	ns	W005	0 0 1 2 1	sic

3845. C₁₈H₁₂N₂

2,2'-Biquinoline

2,2'-Biquinolyl

RN: 119-91-5**MP (°C):** 193**MW:** 256.31**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-06	1.020E-03	24	H106	1 0 2 2 2	
3.980E-06	1.020E-03	24	M303	1 0 1 1 2	

3846. C₁₈H₁₂N₄O

4-Hydroxy-6,7-diphenylpteridine

4-Hydroxy-6:7-diphenylpteridine

RN: 102943-71-5**MP (°C):****MW:** 300.32**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.658E-04	2.000E-01	20	A019	2 2 1 1 2	

3847. C₁₈H₁₃ClFN₃

Midazolam

8-Chloro-6-(*o*-fluorophenyl)-1-methyl-4H-imidazo[1,5-a][1,4]benzodiazepine**RN:** 59467-70-8**MP (°C):****MW:** 325.78**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.658E-04	5.400E-02	24	A404	2 0 2 2 2	intrinsic pH = 9.5

3848. C₁₈H₁₃ClF₃NO₂

Fluoroglycofen-ethyl

Super Blazer

Fluoroglycofen ethyl ester

Ethoxycarbonylmethyl-5-(2-chloro-4-trifluoromethylphenoxy)-2-nitrobenzoate-

hyphen-ethoxy-2-oxoethyl 5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoate

5-[2-Chloro-4-(trifluoromethyl)-phenoxy]-2-nitro-benzoic acid 2-ethoxy-2-oxoethyl ester

RN: 77501-90-7**MP (°C):****MW:** 447.76**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.349E-06	6.040E-04	ns	R427	0 0 0 0 0	

3849. C₁₈H₁₃N

6-Aminochrysene

6-Chrysenamine

RN: 2642-98-0

MP (°C): 210

MW: 243.31

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.370E-07	1.550E-04	24	H106	1 0 2 2 2	
6.370E-10	1.550E-07	ns	M349	0 2 1 1 2	

3850. C₁₈H₁₃NO₃

Furo[3,4-b]quinolin-3(1H)-one, 9-hydroxy-6-methyl-1-phenyl-

RN: 74103-08-5 MP (°C):

MW: 291.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.463E-08	1.300E-05	25	P089	0 0 0 0 0	
1.270E-07	3.700E-05	37	P089	0 0 0 0 0	
2.163E-07	6.300E-05	51	P089	0 0 0 0 0	

3851. C₁₈H₁₃NO₃

N-1-Naphthylphthalamic acid

Naptalam

2-((1-Naphthylamino)carbonyl)benzoic acid

Naphthylphthalamic acid

ALANAP-1

NPA

RN: 132-66-1 MP (°C): 185

MW: 291.31 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.866E-04	2.000E-01	25	B200	1 0 0 0 2	
6.866E-04	2.000E-01	ns	B185	0 0 0 0 0	
6.866E-04	2.000E-01	ns	N013	0 0 0 0 2	
6.866E-04	2.000E-01	rt	M161	0 0 0 0 2	

3852. C₁₈H₁₄

o-Terphenyl

1,2-Diphenyl benzene

RN: 84-15-1

MP (°C): 58

MW: 230.31

BP (°C): 332

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.380E-06	1.239E-03	25	A325	2 1 2 2 2	

3853. C₁₈H₁₄

m-Terphenyl
1,3-Diphenyl benzene

RN: 92-06-8 **MP (°C):** 89
MW: 230.31 **BP (°C):** 365

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.560E-06	1.511E-03	25	A325	2 1 2 2 2	

3854. C₁₈H₁₄

p-Terphenyl
1,4-Diphenyl benzene

RN: 92-94-4 **MP (°C):** 213
MW: 230.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.800E-08	1.796E-05	25	A325	2 1 2 2 1	

3855. C₁₈H₁₄Cl₄N₂O

Miconazole

1-[2-(2,4-Dichlorophenyl)-2-[(2,4-dichlorophenyl)methoxy]ethyl]-1H-imidazole

1-[2,4-Dichloro-β-[(2,4-dichlorobenzyl)oxy]phenethyl]imidazole

Conoderm

RN: 22916-47-8 **MP (°C):**
MW: 416.14 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.80E-09	<2.00E-06	25	P348	0 0 0 0 0	
2.163E-04	9.000E-02	amb	L434	0 0 0 0 0	

3856. C₁₈H₁₄N₄O

Disperse yellow 23

Phenol, 4-[[4-(phenylazo)phenyl]azo]-
p-Hydroxy-*p*-bis(azobenzene)

RN: 6250-23-3 **MP (°C):**
MW: 302.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-10	6.047E-08	25	B333	0 0 0 0 0	
1.300E-07	3.930E-05	71.8	D093	1 2 1 2 0	EFG
5.500E-07	1.663E-04	84.1	D093	1 2 1 2 0	EFG
2.300E-06	6.954E-04	97.4	D093	1 2 1 2 0	EFG

3857. C₁₈H₁₄N₄O₂

Disperse orange 1

Dye VI

C.I. Disperse orange 1

4-(*p*-Nitrophenylazo)diphenylamine

4-Anilino-4'-nitroazobenzene

4-(4-Nitrophenylazo)diphenylamine

RN: 2581-69-3 **MP (°C):** 157**MW:** 318.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-09	4.775E-07	25	B333	0 0 0 0 0	
3.000E-07	9.550E-05	84.10	B198	1 2 1 1 0	
1.420E-06	4.520E-04	97.40	B198	1 2 1 1 2	
4.900E-06	1.560E-03	111.60	B198	1 2 1 1 1	
1.950E-05	6.208E-03	127	B198	1 2 1 1 2	

3858. C₁₈H₁₄N₄O₅S

Sulfasalazine

Salicylazosulfapyridine

SASP

Sulcolon

Salazosulfapyridine

Salicylazosulfapyridine

RN: 599-79-1 **MP (°C):** 240–245**MW:** 398.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.510E-05	1.000E-02	ns	K444	0 0 0 0 0	

3859. C₁₈H₁₅Cl₃N₂O

Econazole

1-[2-[(4-Chlorophenyl)methoxy]-2-(2,4-dichlorophenyl)ethyl]-1H-imidazole

RN: 27220-47-9 **MP (°C):****MW:** 381.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.694E-04	3.700E-01	amb	L434	0 0 0 0 0	

3860. C₁₈H₁₅Cl₄N₃O₄

Miconazole nitrate-β cyclodextrin complexant

RN: 22832-87-7 **MP (°C):****MW:** 479.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-04	1.773E-01	25	P348	0 0 0 0 0	

3861. C₁₈H₁₅NO₃

Oxaprozin

4,5-Diphenyl-2-oxazolepropanoic acid

4,5-Diphenyl-2-oxazole-propionic acid

Choledyl

Daypro

Oxaprozin

RN: 21256-18-8 **MP (°C):****MW:** 293.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.364E-05	4.000E-03	37	Y421	0 0 0 0 0	

3862. C₁₈H₁₅N₃O₅

1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, methyl ester

RN: 104663-14-1 **MP (°C):** 156.5**MW:** 353.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.981E-05	7.000E-03	21	N337	0 0 0 0 0	pH 5
1.900E-05	6.713E-03	21	N337	0 0 0 0 0	pH 5

3863. C₁₈H₁₅O₄P

Triphenyl phosphate

Phosphoric acid triphenyl ester

Triphenyl phosphoric acid ester

Phenyl phosphate

TPP

RN: 115-86-6 **MP (°C):** 49**MW:** 326.29 **BP (°C):** 245

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.237E-06	7.300E-04	24	H116	2 1 0 0 2	
6.129E-05	2.000E-02	ns	F014	0 0 0 0 0	

3864. C₁₈H₁₆ClNO₅Fenoxyprop-*p*-ethylFenoxyprop-*p* ethyl ester

Propanoic acid

2-{4-[(6-Chloro-2-benzoxazolyl)oxy]phenoxy}-ethyl ester

RN: 71283-80-2 **MP (°C):****MW:** 361.78 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.950E-06	7.054E-04	ns	R427	0 0 0 0 0	

3865. C₁₈H₁₆Cl₃N₃O₄

Econazole nitrate

Pevaryl

Spectazole

R 14827

RN: 68797-31-9 MP (°C):

MW: 444.70 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-03	7.115E-01	25	P348	0 0 0 0 0	

3866. C₁₈H₁₆N₂O₃

Benzoyltryptophan

N-Benzoyl-DL-tryptophan

RN: 2901-79-3 MP (°C):

MW: 308.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.816E-03	5.600E-01	25.1	N026	0 0 0 0 0	

3867. C₁₈H₁₆N₄O₃S

2-(N4-Acetylulfanilylamino)-4-phenylpyrimidine

RN: MP (°C):

MW: 368.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.772E-06	3.600E-03	37	R076	1 2 0 0 1	

3868. C₁₈H₁₇ClN₄O₆.0.5H₂O

9-[5-O-(4-Chlorobenzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine (hemihydrate)

RN: 121032-34-6 MP (°C): 122–124

MW: 429.82 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.880E-04	8.081E-02	37	M378	1 2 1 1 2	pH 7.2

3869. C₁₈H₁₇Cl₂NO₃

Benzoylprop-ethyl

Ethyl *N*-benzoyl-*N*-(3,4-dichlorophenyl)-2-aminopropionate

FX 2182

N-Benzoyl-*N*-(3,4-dichlorophenyl)-DL-alanine ethyl ester

Enaven

Suffix

RN: 22212-55-1 **MP (°C):** 70.5**MW:** 366.25 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.461E-05	2.000E-02	25	M161	1 0 0 0 1	

3870. C₁₈H₁₇N₅O₈6-Methoxy-9-(5-*O*-[4-nitrobenzoyl]-β-D-arabinofuranosyl)-9H-purine**RN:** 121032-21-1 **MP (°C):** 202–203**MW:** 431.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-05	1.467E-02	37	M378	1 2 1 1 2	pH 7.2

3871. C₁₈H₁₈CINO₄

Clanobutin

Butanoic acid, 4-[(4-chlorobenzoyl)(4-methoxyphenyl)amino]-

Bykahepar

RN: 30544-61-7 **MP (°C):****MW:** 347.80 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.270E-04	4.417E-02	37	K093	1 2 1 1 2	pH 3.0

3872. C₁₈H₁₈CINO₅

Etofibrate

3-Pyridinecarboxylic acid, 2-[2-(4-chlorophenoxy)-2-methyl-1-oxopropoxy]ethyl ester

Tricerol

Lipo-Merz

RN: 31637-97-5 **MP (°C):****MW:** 363.80 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	7.276E-03	rt	G093	0 1 1 1 2	pH4

3873. C₁₈H₁₈CINO₅

Benzoximate

RN: 29104-30-1 **MP (°C):** 73
MW: 363.80 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.318E-05	3.026E-02	ns	R427	0 0 0 0 0	

3874. C₁₈H₁₈CINS

Chlorprothixene

Taractan

1-Propanamine, 3-(2-chloro-9H-thioxanthen-9-ylidene)-N,N-dimethyl-, (3Z)-
 Rentovet

RN: 113-59-7 **MP (°C):**
MW: 315.87 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.936E-05	1.243E-02	20	H301	0 0 0 0 0	
1.221E-06	3.858E-04	22.5	B440	0 0 0 0 0	

3875. C₁₈H₁₈N₂O₄

C.I. Disperse blue 23

1,4-bis[(2-Hydroxyethyl)amino]anthraquinone
 Acetoquinone blue BF

RN: 4471-41-4 **MP (°C):** 248
MW: 326.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-06	7.833E-04	25	B333	0 0 0 0 0	

3876. C₁₈H₁₈N₄O₆

9-[5-O-(Benzoyl-β-D-arabinofuranosyl)]-6-methoxy-9H-purine

RN: 121032-31-3 **MP (°C):** 202–204
MW: 386.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-05	2.859E-02	37	M378	1 2 1 1 2	pH 7.2

3877. C₁₈H₁₈N₄O₆.0.75H₂O

2'-Benzoyl-6-methoxypurine arabinoside (0.75 hydrate)

RN: 145913-44-6 MP (°C): 84–86

MW: 399.88 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.780E-02	7.118E+00	37	C348	0 0 0 0 0	pH 7.00

3878. C₁₈H₁₈N₈O₆

7,7'-Succinylidetheophylline

RN: 58447-18-0 MP (°C):

MW: 442.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.630E-03	7.211E-01	25	L067	1 0 1 1 2	

3879. C₁₈H₁₈O₂

Dienestrol

3,4-bis(4-Hydroxyphenyl)-2,4-hexadiene

Dehydrostilbestrol

RN: 84-17-3 MP (°C): 227.5

MW: 266.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.126E-05	3.000E-03	37	B039	2 1 1 1 0	EFG
1.122E-05	2.988E-03	ns	R427	0 0 0 0 0	

3880. C₁₈H₁₈O₂

Equilenin

3-Hydroxy-17-keto-δ(1,3,5-10,6,8)estrapentaene

1,3,5-10,6,8-Estrapentaen-3-ol-17-one

RN: 517-09-9 MP (°C): 258

MW: 266.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.707E-06	1.520E-03	25	L033	1 0 2 1 2	

3881. C₁₈H₁₈O₃

Flurecol-butyl

Flurenol-*n*-butyl ester*n*-Butyl-9-hydroxyfluorene-(9)-carboxylate

RN: 2314-09-2 MP (°C): 70

MW: 282.34 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.293E-02	3.650E+00	20	B200	1 0 0 0 2	<i>sic</i>
1.293E-04	3.650E-02	20	M161	1 0 0 0 2	<i>sic</i>

3882. C₁₈H₁₉Cl₂NO₄

Felodipine

3,5-Pyridinedicarboxylic acid, 4-(2,3-dichlorophenyl)-1,4-dihydro-2,6-dimethyl-, ethyl methyl ester

Plendil

RN: 72509-76-3 MP (°C):

MW: 384.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.301E-06	5.000E-04	20	N322	0 0 0 0 0	
1.179E-05	4.530E-03	22	M382	2 1 1 1 1	

3883. C₁₈H₁₉F₃N₂S4-Trifluoromethyl-*N,N*-dimethyl-10H-phenothiazine-10-propanamide

RN: 3852-94-6 MP (°C):

MW: 352.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-06	2.467E-03	ns	G023	0 0 1 1 0	

3884. C₁₈H₁₉F₃N₂S

Fluopromazine

Triflupromazine

RN: 146-54-3 MP (°C): <25

MW: 352.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.762E-03	24	G022	2 0 1 1 1	
5.000E-06	1.762E-03	ns	F027	0 0 0 0 0	

3885. C₁₈H₁₉NO

Desmethyldoxepin

1-Propanamine, 3-dibenz[b,e]oxepin-11(6H)-ylidene-*N*-methyl-**RN:** 1225-56-5 **MP (°C):****MW:** 265.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.950E-04	1.048E-01	25	E051	1 0 2 1 2	

3886. C₁₈H₁₉N₂O₄

N-Benzoyl-L-tyrosinamide acetate

RN: **MP (°C):****MW:** 327.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-04	4.256E-02	25	A066	1 0 1 1 1	

3887. C₁₈H₁₉N₃O₆S

Cephaloglycin

5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid

RN: 3577-01-3 **MP (°C):****MW:** 405.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.590E-02	1.050E+01	25	P311	0 0 0 0 0	EFG

3888. C₁₈H₁₉N₅O₃

C.I. Disperse dye

Propanenitrile, 3-[(2-hydroxyethyl)[3-methyl-4-[(4-nitrophenyl)azo]phenyl]amino]-

Celliton discharge scarlet RNL

Celliton fast scarlet RN

RN: 6054-58-6 **MP (°C):** 156**MW:** 353.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-07	6.714E-05	25	B333	0 0 0 0 0	

3889. C₁₈H₁₉N₅O₆.0.3H₂O9-[5-*O*-(4-Aminobenzoyl- β -D-arabinofuranosyl)]-6-methoxy-9H-purine (0.3 hydrate)**RN:** 121032-39-1 **MP (°C):** 198–200**MW:** 406.79 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-05	1.383E-02	37	M378	1 2 1 1 2	pH 7.2

3890. C₁₈H₁₉N₅O₆2'-(*o*-Aminobenzoyl)-6-methoxypurine arabinoside

RN: 121032-55-1 MP (°C):

MW: 401.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.060E-02	8.268E+00	37	C348	0 0 0 0 0	pH 7.00

3891. C₁₈H₂₀

2,4-Diphenyl-4-methyl-2-pentene

RN: 6362-80-7 MP (°C):

MW: 236.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-07	2.475E-05	ns	D001	0 0 0 0 2	

3892. C₁₈H₂₀Cl₂O₂1-Dichloro-2,2-bis(*p*-ethoxyphenyl)ethane

RN: 7388-32-1 MP (°C):

MW: 339.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.664E-08	2.600E-05	rt	C122	0 0 0 0 0	

3893. C₁₈H₂₀N₄O₇S2'-(*p*-Methylbenzenesulfonyl)-6-methoxypurine arabinoside

RN: 145913-49-1 MP (°C): 214–215

MW: 436.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.240E-04	5.412E-02	37	C348	0 0 0 0 0	pH 7.00

3894. C₁₈H₂₀O₂

Equilin

3-Hydroxy-17-keto- δ (1,3,5-10,7)estratetraene

1,3,5(10),7-Estratetraen-3-ol-17-one

RN: 474-86-2 MP (°C): 238

MW: 268.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.217E-06	1.400E-03	25	H049	0 0 0 0 0	
5.254E-06	1.410E-03	25	L033	1 0 2 1 2	

3895. C₁₈H₂₀O₂

Diethylstilbestrol

Diethylstilboestrol

Destrol

4,4'-(1,2-Diethyl-1,2-ethenediyl)bisphenol

Tylosterone

Vagestrol

RN: 56-53-1**MP (°C):** 169**MW:** 268.36**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.472E-05	1.200E-02	25	G009	1 0 1 1 1	
9.316E-05	2.500E-02	30	M007	2 2 1 2 2	average of 6

3896. C₁₈H₂₁CIN₂

Chlorcyclizine

Chlorcyclizine

RN: 82-93-9**MP (°C):****MW:** 300.83**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-03	3.008E-01	37.5	L034	2 2 0 1 2	pH 7.4

3897. C₁₈H₂₁CIN₂S2-Chloro-*N,N*-dimethyl-10H-phenothiazine-10-butanamine**RN:** 13094-23-0**MP (°C):****MW:** 332.90**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.664E-03	ns	G023	0 0 1 1 0	

3898. C₁₈H₂₁ClO1-Chloro-1-methyl-2-(*p*-methylphenyl)-2-*p*-ethoxyphenyl)ethane**RN:** 56265-27-1**MP (°C):****MW:** 288.82**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.540E-06	1.600E-03	rt	C122	0 0 0 0 0	

3899. C₁₈H₂₁NO₃

Codeine

Codein

Methylmorphin

7,8-Didehydro-4,5- α -epoxy-3-methoxy-17-methylmorphinan-6- α -ol

Nucofed

Robitussin AC

RN: 76-57-3**MP (°C):** 155**MW:** 299.37**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.006E-02	9.000E+00	20	A073	1 1 1 1 0	
2.672E-02	8.000E+00	20	F300	1 0 0 0 0	
2.760E-02	8.264E+00	20	K052	1 1 1 1 2	
1.591E-01	4.762E+01	25	E041	2 2 2 2 0	EFG, form III, recrystallized
3.242E-02	9.705E+00	25	E041	2 2 2 2 0	EFG, form II, recrystallized
3.176E-02	9.509E+00	25	E041	2 2 2 2 0	EFG, form I, recrystallized
3.571E-02	1.069E+01	25	R338	0 0 0 0 0	
3.340E-02	1.000E+01	30	A073	1 1 1 1 1	
3.674E-02	1.100E+01	40	A073	1 1 1 1 1	
4.342E-02	1.300E+01	50	A073	1 1 1 1 1	
5.010E-02	1.500E+01	60	A073	1 1 1 1 1	
6.013E-02	1.800E+01	70	A073	1 1 1 1 1	
6.347E-02	1.900E+01	80	A073	1 1 1 1 1	
5.578E-02	1.670E+01	80	F300	1 0 0 0 2	
8.017E-02	2.400E+01	90	A073	1 1 1 1 1	
1.069E-01	3.200E+01	100	A073	1 1 1 1 1	

3900. C₁₈H₂₁NO₃

Thebainone A

Morphinan-6-one, 7,8-didehydro-4-hydroxy-3-methoxy-17-methyl-Thebainon

RN: 467-98-1**MP (°C):** 146**MW:** 299.37**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.336E-02	4.000E+00	20	F300	1 0 0 0 0	
2.839E-02	8.500E+00	100	F300	1 0 0 0 1	

3901. C₁₈H₂₁NO₃·H₂O

Codeine (monohydrate)

Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-methoxy-17-methyl-, monohydrate, (5 α ,6 α)**RN:** 6059-47-8 **MP (°C):** 155**MW:** 317.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.604E-02	8.264E+00	c	D004	0 0 0 0 0	

3902. C₁₈H₂₁NO₄2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-(dimethylamino)-2-oxoethyl ester, (*S*)Naproxen, *N,N*-dimethyl glycolamide ester2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-(dimethylamino)-2-oxoethyl esterNaproxen *N,N*-dimethyl glycolamide ester**RN:** 114665-18-8 **MP (°C):** 150.5**MW:** 315.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.268E-05	4.000E-03	21	B331	1 2 2 1 2	pH 7.4
1.268E-05	4.000E-03	21	B331	0 0 0 0 0	

3903. C₁₈H₂₂CINO₄

Oxycodone hydrochloride

4,5-Epoxy-14-hydroxy-3-methoxy-17-methylmorphinan-6-one hydrochloride

Endocet

Percocet

Supeudol

Roxicet

RN: 124-90-3 **MP (°C):** 270–271**MW:** 351.83 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.060E-01	1.429E+02	ns	S469	0 0 0 0 0	

3904. C₁₈H₂₂N₂

1-(Diphenylmethyl)-4-methylpiperazine

RN: **MP (°C):****MW:** 266.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.962E-04	1.855E-01	25	M438	0 0 0 0 0	

3905. C₁₈H₂₂N₄O₅

Dis. A. 9

Ethanol, 2,2'-[[4-[(2-methoxy-4-nitrophenyl)azo]-3-methylphenyl]imino]bis-4-[bis(2-Hydroxyethyl)amino]-2'-methoxy-2-methyl-4'-nitroazobenzene

RN: 41541-11-1 **MP (°C):****MW:** 374.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.500E-06	1.685E-03	25	B333	0 0 0 0 0	

3906. C₁₈H₂₂O₂

Hexestrol

4,4'-(1,2-Diethylethylene)diphenol

Dihydrodiethylstilbestrol

Esestrolo

RN: 5635-50-7 **MP (°C):** 186.5**MW:** 270.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.438E-05	1.200E-02	37	B039	2 1 1 1 0	EFG
3.699E-05	1.000E-02	37	B045	1 0 1 1 1	
4.365E-05	1.180E-02	ns	R427	0 0 0 0 0	

3907. C₁₈H₂₂O₂

Estrone

Oestrone

Folliculin

1,3,5(10)-Estratrien-3-ol-17-one

Estra-1,3,5(10)-Trien-17-one, 3-hydroxy-

Oestrin

RN: 53-16-7 **MP (°C):** 252.5**MW:** 270.37 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.659E-06	1.530E-03	22	Y419	0 0 0 0 0	
2.959E-06	8.000E-04	25	H049	0 0 0 0 0	
1.110E-04	3.000E-02	25	I309	0 0 0 0 0	<i>sic</i>
2.959E-06	8.000E-04	25	L033	1 0 2 1 1	
1.109E-03	2.999E-01	25	P324	0 0 0 0 0	
4.808E-06	1.300E-03	25	S468	0 0 0 0 0	
8.200E-06	2.217E-03	37	H034	1 0 2 1 1	pH 7.4
1.184E-05	3.200E-03	37	L010	2 0 2 1 1	
3.162E-06	8.550E-04	ns	A074	0 0 0 0 0	EFG

3908. C₁₈H₂₃NO

Orphenadrine

Disipal

Marflex

Noradex

Orflagen

Norflex

RN: 83-98-7**MP (°C):****MW:** 269.39**BP (°C):** 195 at 12 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.686E-06	1.801E-03	22.5	B440	0 0 0 0 0	

3909. C₁₈H₂₃N₃O₅S

L-Leu-dapsone

2-Amino-N-[4-[(4-aminophenyl)sulfonyl]phenyl]-4-methyl-, (S)-

Pentanamide

RN: 160349-00-8 **MP (°C):****MW:** 361.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.576E-04	3.100E-01	25	P351	0 0 0 0 0	pH 7.4
>6.92E-02	>2.50E+01	25	P351	0 0 0 0 0	

3910. C₁₈H₂₃N₃O₄S

Phentolamine methanesulfonate

Vasomax

Regitine mesylate

Regitine methanesulfonate

RN: 65-28-1 **MP (°C):** 177**MW:** 377.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.979E+00	1.502E+03	30	D011	1 0 1 0 2	

3911. C₁₈H₂₄I₃N₃O₉

1,3-Benzenedicarboxamide, 5RS-[(2,3-dihydroxy-1-oxobutyl)amino]-N,N'-bis(2,3-dihydroxypropyl)-2,4,6-triiodo-[RS-(RS*,S*)]-

RN: 77868-48-5 **MP (°C):****MW:** 807.12 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.327E-01	1.071E+02	25	P091	0 0 0 0 0	

3912. C₁₈H₂₄N₄O₂

2,5-Diaziridinyl-3,6-dipyrrolidino-1,4-benzoquinone

RN: 59886-43-0 MP (°C): 160

MW: 328.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.522E-03	5.000E-01	rt	C317	0 0 0 0 0	

3913. C₁₈H₂₄N₄O₂S

2-Sulfanilamido-5,6,7,8,-tetrahydro-8-isopropyl-5-methyl-quinazoline

RN: 71119-36-3 MP (°C): 185-187

MW: 360.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.658E-05	2.400E-02	29	C049	0 0 0 0 0	

3914. C₁₈H₂₄N₄O₂S

2-Sulfanilamidobornyleneepyrimidine

RN: MP (°C): 276

MW: 360.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.322E-05	3.000E-02	29	C049	0 0 0 0 0	

3915. C₁₈H₂₄N₄O₃S

L-Lys-dapsone

Hexanamide, 2,6-diamino-N-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (S)

RN: 160349-03-1 MP (°C):

MW: 376.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.73E-01	>6.50E+01	25	P351	0 0 0 0 0	pH 7.4
>1.73E-01	>6.50E+01	25	P351	0 0 0 0 0	

3916. C₁₈H₂₄O₂

Estradiol

17-β-Estradiol

Estradiol-17β

RN: 50-28-2 MP (°C): 176

MW: 272.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.652E-05	4.500E-03	20	G072	1 2 2 1 2	

(continued)

3916. C₁₈H₂₄O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-06	1.689E-03	20	L077	1 2 2 2 1	
1.413E-05	3.850E-03	22	Y419	0 0 0 0 0	
2.566E-05	6.990E-03	23	B014	0 0 1 2 2	
7.413E-06	2.019E-03	25	B041	1 0 2 2 0	EFG
6.000E-07	1.634E-04	25	E014	2 2 2 1 1	pH 7.3
1.432E-05	3.900E-03	25	H049	0 0 0 0 0	
1.836E-05	5.000E-03	25	K003	2 1 1 1 1	
5.544E-06	1.510E-03	25	S468	0 0 0 0 0	
1.320E-05	3.596E-03	27.34	L077	1 2 2 2 2	
2.060E-05	5.611E-03	35	L077	1 2 2 2 2	
1.500E-05	4.086E-03	37	H034	1 0 2 1 2	pH 7.4
2.350E-05	6.401E-03	37	H035	1 1 1 1 2	pH 7.4
1.430E-05	3.895E-03	37	H054	0 0 0 0 0	
1.880E-05	5.120E-03	37	R069	0 0 0 0 0	pH 7.4
1.000E-05	2.724E-03	37.50	B041	1 0 2 2 0	EFG
2.830E-05	7.709E-03	42	L077	1 2 2 2 2	
3.560E-05	9.697E-03	50	L077	1 2 2 2 2	

3917. C₁₈H₂₄O₂ α -Estradiol17- α -Estradiol

RN: 57-91-0

MP (°C): 220

MW: 272.39

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.432E-05	3.900E-03	25	L033	1 0 2 1 2	

3918. C₁₈H₂₄O₃

Estriol

Oestriol

Drihydroxyestrin

RN: 50-27-1

MP (°C): 284.5

MW: 288.39

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.047E-04	3.020E-02	22	Y419	0 0 0 0 0	
1.110E-05	3.200E-03	25	H049	0 0 0 0 0	
1.000E-04	2.884E-02	30	O321	0 0 0 0 0	
1.006E-04	2.900E-02	30	O321	0 0 0 0 0	

3919. C₁₈H₂₄O₆

Butylphthalyl butyl glycolate

1,2-Benzenedicarboxylic acid 2-butoxy-2-oxoethyl butyl ester

Butyl carbobutoxymethyl phthalate

RN: 85-70-1 **MP (°C):** <-35**MW:** 336.39 **BP (°C):** 219

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.567E-05	1.200E-02	20	F070	1 0 0 0 2	

3920. C₁₈H₂₅I₃N₃O₉

3,5-Diacetylamino-2,4,6-triiodobenzoic acid methyl-glucamide

RN: **MP (°C):** 191**MW:** 808.13 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.101E+00	8.900E+02	20	L100	1 0 0 0 1	

3921. C₁₈H₂₅NO

Racemethorphan

Dextromethorphan HBr

RN: 510-53-2 **MP (°C):****MW:** 271.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.326E-01	3.600E+01	37	F008	1 1 2 2 2	0.1N HCl

3922. C₁₈H₂₅NO

Dextromethorphan

(+) -*cis*-1,3,4,9,10,10a-Hexahydro-6-methoxy-11-methyl-2H-10,4a-iminoethanophenanthrene

Romilar CF

DXM Free Base

3-Methoxy-17-methyl-(9 α ,13 α ,14 α)-morphinan

Benylin DM

RN: 125-71-3 **MP (°C):****MW:** 271.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.316E-04	9.000E-02	amb	L434	0 0 0 0 0	

3923. C₁₈H₂₅NO₅S₂

Methyl N-{5-[(3R)-1,2-dithiolan-3-yl]-pentanoyl}-L-tyrosinate

RN: MP (°C):
MW: 399.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.003E-05	1.200E-02	ns	S453	0 0 0 0 0	

3924. C₁₈H₂₅N₃O₂

2-Ethoxy-N-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide

N-[2-(Diethylamino)ethyl]-2-ethoxyquinoline-4-carboxamide

RN: 2716-99-6 **MP (°C):**
MW: 315.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.600E-04	2.082E-01	ns	M066	0 0 0 0 1	

3925. C₁₈H₂₆NO₄

Ibuprofen N-methyl-N-carbamoyl methyl glycolamide ester

RN: MP (°C): 100.5
MW: 320.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.057E-04	1.300E-01	0	B331	1 2 2 1 1	pH 7.4

3926. C₁₈H₂₆N₂O₄

Benzeneacetic acid, β-methyl-4-(2-methylpropyl)-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester

Ibuprofen N-methyl-N-carbamoyl methyl glycolamide ester

RN: 114665-11-1 **MP (°C):** 100–101
MW: 334.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-04	1.300E-01	21	B331	0 0 0 0 0	

3927. C₁₈H₂₆N₄O₆

9-[5-O-(Heptylate-β-D-arabinofuranosyl)]-6-methoxy-9H-purine

RN: 142963-79-9 **MP (°C):** foam
MW: 394.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.120E-04	8.362E-02	37	M378	1 2 1 1 2	pH 7.2

3928. C₁₈H₂₆N₄O₆.0.5H₂O

2'-Heptanyl-6-methoxypurine arabinoside (hemihydrate)

RN: 145913-40-2 MP (°C): 83–85

MW: 403.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.780E-03	1.122E+00	37	C348	0 0 0 0 0	pH 7.00

3929. C₁₈H₂₆O

Acetyl ethyl tetramethyl tetralin

1-(3-Ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthalenyl)ethanone

AETT

1,1,4,4-Tetramethyl-6-ethyl-7-acetyl-1,2,3,4-tetrahydronaphthalene

Ethanone, 1-(3-ethyl-5,6,7,8-tetrahydro-5,5,8,8-tetramethyl-2-naphthyl)-

RN: 88-29-9 MP (°C):

MW: 258.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.644E-08	1.200E-05	ns	B338	0 0 0 0 1	

3930. C₁₈H₂₆O₂

Nortestosterone

Estr-4-en-3-one, 17-hydroxy-, (17 β)

RN: 434-22-0 MP (°C):

MW: 274.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.126E-02	3.090E+00	25	P324	0 0 0 0 0	

3931. C₁₈H₂₆O₄

Dipentyl phthalate

Diethyl phthalate

RN: 131-18-0 MP (°C): <-55

MW: 306.41 BP (°C): 342

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.450E-06	4.443E-04	20	L300	2 1 0 2 2	
9.791E-07	3.000E-04	25	F067	1 0 2 2 0	
3.263E-04	9.999E-02	ns	F014	0 0 0 0 0	

3932. C₁₈H₂₆O₆

Butyl phthalyl butyl glycollate

RN: **MP (°C):**
MW: 338.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.955E-05	1.000E-02	15	H069	1 0 1 1 0	
5.318E-04	1.800E-01	ns	F014	0 0 0 0 1	

3933. C₁₈H₂₇NO

N-Nonylcinnamamide

2-Propenamide, *N*-nonyl-3-phenyl-
RN: 59832-01-8 **MP (°C):**
MW: 273.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.220E-06	6.070E-04	ns	H350	0 0 0 0 0	

3934. C₁₈H₂₇NO₃*p*-Acetamidophenyl decanoate

Acetaminophen decanoate

RN: 54942-37-9 **MP (°C):** 107
MW: 305.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.947E-05	9.000E-03	25	B010	1 1 1 1 0	

3935. C₁₈H₂₇NO₃

Capsaicin

Nonenamide, *N*-(4-hydroxy-3-methoxyphenyl)methyl)-8-methyl-, (E)-Zostrix

RN: 404-86-4 **MP (°C):** 63 C
MW: 305.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	3.176E-02	27	Z412	0 0 0 0 0	

3936. C₁₈H₂₇N₅O₅9-[S'-(*O*-Caprylyl)-β-D-arabinofuranosyl]adenine ester

RN: 66460-51-3 **MP (°C):**
MW: 393.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.542E-04	1.000E-01	ns	B134	0 1 1 1 0	

3937. C₁₈H₂₈N₂O

DL-Bupivacaine

Bupivacaine

Marcaine

Bupivacaine

Marcaine (hydrochloride monohydrate)

RN: 2180-92-9 **MP (°C):** 107**MW:** 288.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-04	1.082E-01	14.9	N046	2 0 1 1 2	intrinsic
9.025E-06	2.603E-03	22.5	B440	0 0 0 0 0	
1.733E-03	5.000E-01	23	F176	2 0 0 2 0	EFG, pH 7.4, intrinsic
3.520E-04	1.015E-01	25	D401	1 2 2 2 2	
3.180E-04	9.172E-02	25	N046	2 0 1 1 2	intrinsic
3.130E-04	9.028E-02	34.5	N046	2 0 1 1 2	intrinsic
4.170E-04	1.203E-01	37	N044	2 1 1 2 2	intrinsic

3938. C₁₈H₂₈N₄O₂

2,5-Diaziridinyl-3,6-bis(butylamino)-1,4-benzoquinone

RN: 59886-48-5 **MP (°C):** 95**MW:** 332.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.01E-04	<1.00E-01	rt	C317	0 0 0 0 0	

3939. C₁₈H₂₈O₃Undecyl *p*-hydroxybenzoate

Undecyl 4-hydroxybenzoate

RN: 69679-31-8 **MP (°C):****MW:** 292.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.079E-03	2.362E+00	25	D081	1 2 2 1 2	

3940. C₁₈H₂₉NO₂

Penbutolol

Levatol

2-Propanol, 1-(2-cyclopentylphenoxy)-3-[(1,1-dimethylethyl)amino]-, (*S*)-**RN:** 38363-40-5 **MP (°C):** 70**MW:** 291.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.402E-02	7.000E+00	rt	H096	1 0 0 0 0	

3941. C₁₈H₂₉NO₃

4-Pentoxybenzoic acid-2-(diethyl-amino)ethyl ester

RN: 38973-73-8 MP (°C):

MW: 307.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	1.845E-02	ns	M066	0 0 0 0 1	

3942. C₁₈H₃₀

2-Phenyldodecane

RN: MP (°C):

MW: 246.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	9.858E-07	25	S377	0 0 0 0 0	

3943. C₁₈H₃₀

4-Phenyldodecane

RN: MP (°C):

MW: 246.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.232E-06	25	S377	0 0 0 0 0	

3944. C₁₈H₃₀

5-Phenyldodecane

RN: MP (°C):

MW: 246.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.232E-06	25	S377	0 0 0 0 0	

3945. C₁₈H₃₀

3-Phenyldodecane

RN: MP (°C):

MW: 246.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-09	1.725E-06	25	S377	0 0 0 0 0	

3946. C₁₈H₃₀
6-Phenyldodecane

RN: MP (°C):
MW: 246.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	9.858E-07	25	S377	0 0 0 0 0	

3947. C₁₈H₃₀N₂O₂
4-Pentylaminobenzoic acid-2-(diethylamino)ethyl ester

RN: 16488-56-5 MP (°C):
MW: 306.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	6.435E-02	ns	M066	0 0 0 0 1	

3948. C₁₈H₃₀O₃
4-Octylphenol diethoxylate
2-[2-(*p*-Octylphenoxy)ethoxy]ethanol

RN: 51437-90-2 MP (°C):
MW: 294.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.483E-05	1.320E-02	20.5	A335	0 0 0 0 0	
4.490E-05	1.322E-02	20.5	A335	0 0 0 0 0	

3949. C₁₈H₃₀O₁₅.4H₂O
Triamylose (tetrahydrate)

RN: MP (°C):
MW: 558.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.298E-02	1.283E+01	20	P048	1 2 1 1 1	

3950. C₁₈H₃₁NO₄
Bisoprolol
1-[Isopropylamino]-3-[isopropoxyethoxymethylphenoxy]-2-propanol
ZEβ
Ziac

RN: 66722-44-9 MP (°C):
MW: 325.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.690E-08	5.500E-06	100	M418	0 0 0 0 0	

3951. C₁₈H₃₁O₄P

Butyl octyl phenyl phosphate

RN: 110459-55-7 MP (°C):

MW: 342.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.84E-04	<2.00E-01	25	B070	1 2 0 1 0	

3952. C₁₈H₃₂O₇

Tributyl citrate

Tri-n-butyl citrate

Butyl citrate

RN: 77-94-1 MP (°C): -20

MW: 360.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.664E-04	6.000E-02	15	H069	1 0 1 1 0	
2.219E-04	7.999E-02	ns	F014	0 0 0 0 0	

3953. C₁₈H₃₂O₁₆

Raffinose

6G- α -D-Galactosylsucrose

Melitose

Gossypose

Melitriose

RN: 512-69-6 MP (°C): 80.0

MW: 504.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.556E-02	3.307E+01	.02	H040	1 2 2 2 2	
1.227E-01	6.191E+01	10.00	H040	1 2 2 2 1	
1.879E-01	9.478E+01	16.38	H040	1 2 2 2 2	
1.937E-01	9.772E+01	16.90	H040	1 2 2 2 2	
2.480E-01	1.251E+02	20	D041	1 0 0 0 2	
2.373E-01	1.197E+02	20.00	H040	1 2 2 2 2	
3.192E-01	1.610E+02	24.80	H040	1 2 2 2 2	
4.555E-01	2.298E+02	25	P049	1 0 1 1 1	
3.228E-01	1.628E+02	25.05	H040	1 2 2 2 2	
3.340E-01	1.685E+02	25.50	H040	1 2 2 2 2	
4.227E-01	2.132E+02	30.00	H040	1 2 2 2 2	
6.398E-01	3.227E+02	39.38	H040	1 2 2 2 2	
6.599E-01	3.329E+02	40.00	H040	1 2 2 2 2	
9.217E-01	4.650E+02	50.00	H040	1 2 2 2 2	
1.016E+00	5.125E+02	53.20	H040	1 2 2 2 2	
1.201E+00	6.060E+02	60.00	H040	1 2 2 2 2	
1.239E+00	6.250E+02	61.60	H040	1 2 2 2 2	
1.473E+00	7.430E+02	70.00	H040	1 2 2 2 2	

(continued)

3953. C₁₈H₃₂O₁₆ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.682E+00	8.484E+02	78.00	H040	1 2 2 2 2	
6.518E-02	3.288E+01	.00	H040	1 2 2 2 1	
2.480E-01	1.251E+02	rt	D021	0 0 1 1 2	

3954. C₁₈H₃₂O₁₆.5H₂O

Raffinose (pentahydrate)

6G- α -D-Galactosylsucrose (pentahydrate)

RN: 17629-30-0 MP (°C): 80

MW: 594.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.531E-02	3.288E+01	0	M043	1 0 0 0 1	
1.041E-01	6.191E+01	10	M043	1 0 0 0 1	
2.014E-01	1.197E+02	20	M043	1 0 0 0 2	
3.586E-01	2.132E+02	30	M043	1 0 0 0 2	
5.599E-01	3.329E+02	40	M043	1 0 0 0 2	
7.821E-01	4.650E+02	60	M043	1 0 0 0 2	
1.019E+00	6.060E+02	80	M043	1 0 0 0 2	

3955. C₁₈H₃₄OSn

Cyhexatin

Tricyclohexylhydroxystannane

Tricyclohexyltin hydroxide

Plictran

Dowco 213

RN: 13121-70-5 MP (°C): 196.5

MW: 385.16 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.60E-06	<1.00E-03	25	M161	1 0 0 0 0	
<2.60E-06	<1.00E-03	ns	K138	0 0 0 0 1	

3956. C₁₈H₃₄O₄

Dibutyl sebacate

Di-n-butyl sebacate

Decanedioic acid dibutyl ester

Dibutyl decanedioate

RN: 109-43-3 MP (°C):

MW: 314.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-04	5.000E-02	ns	F014	0 0 0 0 0	

3957. C₁₈H₃₆O₂

Stearic acid
 Stearin saeure
 Octadecanoic acid
RN: 57-11-4 **MP (°C):** 70
MW: 284.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.327E-06	1.800E-03	0	B136	1 0 2 1 1	
9.842E-06	2.800E-03	20	B136	1 0 2 1 1	
1.055E-05	3.000E-03	20	F300	1 0 0 0 0	
1.019E-05	2.900E-03	20.0	R001	1 1 1 1 1	
2.100E-06	5.974E-04	25	J001	1 0 2 1 1	
1.970E-06	5.604E-04	25	R002	0 0 0 0 0	
1.195E-05	3.400E-03	30	B136	1 0 2 1 1	
1.195E-05	3.400E-03	30.0	R001	1 1 1 1 1	
1.700E-05	4.836E-03	35	M004	2 0 0 0 2	
1.476E-05	4.200E-03	45	B136	1 0 2 1 1	
1.476E-05	4.200E-03	45.0	R001	1 1 1 1 1	
2.700E-06	7.681E-04	50	J001	1 0 2 1 1	
5.770E-05	1.641E-02	50	M004	2 0 0 0 2	
1.758E-05	5.000E-03	60	B136	1 0 2 1 1	
1.758E-05	5.000E-03	60	F300	1 0 0 0 0	
1.758E-05	5.000E-03	60.0	R001	1 1 1 1 1	
1.145E-05	3.257E-03	62.5	M004	1 0 0 0 2	
6.327E-06	1.800E-03	.0	R001	1 1 1 1 1	

3958. C₁₈H₃₈

n-Octadecane
 Octadecane
RN: 593-45-3 **MP (°C):** 29.5
MW: 254.50 **BP (°C):** 317.0

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.715E-07	1.200E-04	10	C331	0 0 0 0 0	
2.358E-08	6.000E-06	25	B069	1 0 1 1 1	
2.240E-08	5.700E-06	25	B069	1 0 1 1 1	
5.894E-07	1.500E-04	30	C331	0 0 0 0 0	
6.680E-07	1.700E-04	60	C331	0 0 0 0 0	
3.045E-08	7.750E-06	ns	B003	0 0 0 0 0	
3.045E-08	7.750E-06	ns	B033	0 0 0 0 2	

3959. C₁₈H₃₈O

Octadecanol

Stearyl alcohol

Octadecyl alcohol

Steraffine

RN: 112-92-5**MP (°C):** 61**MW:** 270.50**BP (°C):** 336

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.082E-06	34	K011	1 2 1 1 1	
2.200E-08	5.951E-06	65	K011	1 2 1 1 1	

3960. C₁₈H₃₉N.2H₂O

Octadecylamine (dihydrate)

1-Amino octadecane (dihydrate)

RN: 124-30-1**MP (°C):****MW:** 305.55**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.891E-09	1.800E-06	ns	R037	0 2 2 1 1	

3961. C₁₈H₃₉O₃P

Dibutyl decyl phosphonate

RN: 36378-71-9**MP (°C):****MW:** 334.48**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.98E-04	<2.00E-01	25	B070	1 2 0 1 0	

3962. C₁₈H₃₉O₄P

Dibutyl decyl phosphate

RN: 111440-78-9**MP (°C):****MW:** 350.48**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.85E-04	<1.00E-01	25	B070	1 2 0 1 0	

3963. C₁₈H₃₉O₇P

Tributoxyethyl phosphate

RN: 78-51-3**MP (°C):** -70**MW:** 398.48**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-03	1.100E+00	25	B070	1 2 0 1 1	

3964. C₁₉H₁₂O₆

Dicumarol

3,3'-Methylene-bis(4-hydroxycoumarin)

Dicoumarol

RN: 66-76-2 **MP (°C):** 290**MW:** 336.30 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.352E-05	1.800E-02	25	M457	0 0 0 0 0	
<4.46E-04	<1.50E-01	25	P312	0 0 0 0 0	

3965. C₁₉H₁₃Cl

6-Chloro-10-methyl-1,2-benzanthracene

RN: 188124-97-2 **MP (°C):****MW:** 276.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.613E-08	1.000E-05	27	D003	1 0 0 1 0	

3966. C₁₉H₁₃Cl

4-Fluoro-10-methyl-1,2-benzanthracene

4-FMBA

RN: 2990-70-7 **MP (°C):****MW:** 276.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-08	5.259E-06	22	B062	0 0 0 0 0	

3967. C₁₉H₁₃Cl

3-Fluoro-10-methyl-1,2-benzanthracene

3-FMBA

RN: 20629-50-9 **MP (°C):****MW:** 276.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-08	5.259E-06	22	B062	0 0 0 0 0	

3968. C₁₉H₁₄

10-Methyl-1,2-benzanthracene

RN: 2541-69-7 **MP (°C):** 141**MW:** 242.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.539E-08	1.100E-05	24	H116	2 1 0 0 1	

3969. C₁₉H₁₄

1'-Methyl-1,2-benzanthracene

RN: 2498-77-3 **MP (°C):** 138
MW: 242.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.270E-07	5.500E-05	27	D003	1 0 0 1 2	

3970. C₁₉H₁₄

5-Methylchrysene

RN: 3697-24-3 **MP (°C):** 117.1
MW: 242.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.559E-07	6.200E-05	27	D003	1 0 0 1 1	

3971. C₁₉H₁₄

9-Methyl-1,2-benzanthracene

RN: 2381-16-0 **MP (°C):** 138
MW: 242.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.527E-07	3.700E-05	24	H116	2 1 0 0 1	

3972. C₁₉H₁₄

6-Methylchrysene

RN: 1705-85-7 **MP (°C):** 149
MW: 242.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.682E-07	6.500E-05	27	D003	1 0 0 1 1	

3973. C₁₉H₁₄O₃

Aurin

Rosolic acid

4-[*bis*-(*p*-Hydroxyphenyl)methylene]-2,5-cyclohexadien-1-one

RN: 603-45-2 **MP (°C):**
MW: 290.32 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.128E-03	1.199E+00	rt	D021	0 0 1 1 1	

3974. C₁₉H₁₄O₅S

Phenolsulfonaphthalein

Phenolrot

RN: 143-74-8

MP (°C): >300

MW: 354.38

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.748E-04	3.100E-01	100	F300	1 0 0 0 2	

3975. C₁₉H₁₆O

Triphenylcarbinol

Triphenylmethanol

RN: 76-84-6

MP (°C): 164.2

MW: 260.34

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.500E-03	1.432E+00	25	D007	2 0 1 1 2	

3976. C₁₉H₁₇ClN₂O

Prazepam

Centrax

7-Chloro-1-(cyclopropylmethyl)-1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one

Demetrin

Verstran

RN: 2955-38-6

MP (°C):

MW: 324.81

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	9.095E-03	25	M320	2 2 1 1 2	
		amb	L434	0 0 0 0 0	

3977. C₁₉H₁₇ClN₂O₄

Quizalofop-ethyl

Quizalofop-et

Quizalofop ethyl ester

Targa

Pilot

NC 302

RN: 76578-14-8

MP (°C): 91.7–92.1

MW: 372.81

BP (°C): 220 at 0.2 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.128E-07	3.030E-04	ns	R427	0 0 0 0 0	

3978. C₁₉H₁₇ClN₂O₄

Glafenine

N-(7-Chloro-4-quinolyl)anthranilate2,3-Dihydroxypropyl-*N*-(7-chloro-4-quinolyl)anthranilate**RN:** 3820-67-5 **MP (°C):** 169.5**MW:** 372.81 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.032E-01	3.846E+01	ns	M152	0 0 0 0 0	pH 1.0, intrinsic

3979. C₁₉H₁₇ClN₄

Fenbuconazole

 α -(2-(4-Chlorophenyl)ethyl)- α -phenyl-1*H*-1,2,4-triazole-1-propanenitrile

Enable

RH-7592

Fenethanil

1,2,4-Triazole-1-propanenitrile, α -{2-(4-chlorophenyl)ethyl}- α -phenyl**RN:** 114369-43-6 **MP (°C):****MW:** 336.83 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.888E-07	1.983E-04	ns	R427	0 0 0 0 0	

3980. C₁₉H₁₇N₃O₄S₂

Sugordomycin

RN: 1405-50-1 **MP (°C):****MW:** 415.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.304E-02	9.572E+00	21	M044	2 0 2 2 2	

3981. C₁₉H₁₇N₃O₄S₂

Cephaloridine

Glaxoridin

Keflordin

Loridine

RN: 50-59-9 **MP (°C):** 184**MW:** 415.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>4.81E-02	>2.00E+01	21	M044	2 0 2 2 0	

3982. C₁₉H₁₇N₃O₅

1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, ethyl ester

RN: 153474-30-7 MP (°C): 165.5

MW: 367.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.722E-05	1.000E-02	21	N337	0 0 0 0 0	pH 5
2.700E-05	9.919E-03	21	N337	0 0 0 0 0	pH 5

3983. C₁₉H₁₈

1,2,3,4-Tetrahydro-10-methyl-1,2-benzanthracene

10-Methyl-1,2-cyclohexane anthracene

RN: 6366-18-3 MP (°C): 117

MW: 246.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.786E-07	4.400E-05	27	D003	1 0 0 1 1	

3984. C₁₉H₁₈Cl₂N₂O₂

G-20

p,p-Dichlorophenylbutazone

RN: 4047-57-8 MP (°C):

MW: 377.27 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.386E-04	9.000E-02	ns	B158	0 0 0 0 1	pH 7.0

3985. C₁₉H₁₈N₂O₃

G-23

1-Oxybutylphenylbutazone

3,5-Pyrazolidinedione, 4-butryrl-1,2-diphenyl-

RN: 13167-98-1 MP (°C):

MW: 322.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.722E-04	1.200E-01	ns	B158	0 0 0 0 1	pH 7.0

3986. C₁₉H₁₈N₂O₃

Kebuzone

3,5-Pyrazolidinedione

RN: 853-34-9 MP (°C): 128

MW: 322.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.402E-04	1.742E-01	20	M140	2 0 1 1 1	

3987. C₁₉H₁₉ClFNO₃

Flamprop-isopropyl

Flufenprop-isopropyl

Isopropyl N-benzoyl-N-(3-chloro-4-fluorophenyl)alanine

1-Methylethyl N-benzoyl-N-(3-chloro-4-fluorophenyl)-DL-alanine

RN: 52756-22-6 MP (°C): 56.5

MW: 363.82 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.948E-05	1.800E-02	20	M161	1 0 0 0 0	

3988. C₁₉H₁₉N₇O₆

Folic acid

N-((p-((2-Amino-4-hydroxy-6-pteridinyl)methyl)amino)benzoyl)-L-glutamic acid

Vitamin M

Pteroylglutamic acid

Folcysteine

Folacin

RN: 59-30-3 MP (°C):

MW: 441.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.619E-03	1.597E+00	25	D041	1 0 0 0 1	sic
3.625E-06	1.600E-03	25	D315	0 0 0 0 0	
2.243E-02	9.901E+00	100	D041	1 0 0 0 0	sic
2.265E-04	1.000E-01	ns	K444	0 0 0 0 0	

3989. C₁₉H₂₀ClNO₉

Griseofulvin-4-carboxy-methoxime

RN: MP (°C):

MW: 441.83 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.704E-04	7.529E-02	37	F033	2 0 2 0 2	

3990. C₁₉H₂₀F₃NO₄

Fluazifop-butyl

Butyl 2-((5-trifluoromethyl-2-pyridinyl)oxy)phenoxy)propanoate

Onecide

Fluazifop-butyl

Fluazifop butyl ester

Hache uno super

RN: 69806-50-4 MP (°C): 13

MW: 383.37 BP (°C): 165 at 2.02 mm Hg

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-06	5.366E-04	ns	S460	0 0 0 0 0	

3991. C₁₉H₂₀N₂O

Cinchoninone

Cinchoninon

9-Deoxy-9-oxocinchonine

RN: 14509-68-3 **MP (°C):****MW:** 292.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.498E-04	1.900E-01	20	F300	1 0 0 0 1	

3992. C₁₉H₂₀N₂O₂

Phenylbutazone

1,2-Diphenyl-4-butyl-3,5-dioxopyrazolidine

Butazolidin

Equiphen

Butazone

RN: 50-33-9 **MP (°C):** 107**MW:** 308.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.415E-05	2.595E-02	20	H301	0 0 0 0 0	
4.864E-05	1.500E-02	20	P026	1 0 1 1 1	
1.102E-04	3.400E-02	25	P096	0 0 0 0 0	
1.540E-04	4.750E-02	30	D015	2 0 1 1 0	EFG
1.000E-03	3.084E-01	35	H091	1 2 2 2 1	<i>sic</i>
9.076E-03	2.799E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
7.575E-03	2.336E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
9.362E-03	2.887E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
6.907E-03	2.130E+00	36	I002	2 2 1 1 2	pH 6.95, recrystallized
2.108E-04	6.500E-02	37	D015	2 0 1 1 0	EFG
1.816E-04	5.600E-02	37	E047	1 0 1 1 1	
7.134E-03	2.200E+00	ns	B158	0 0 0 0 1	pH 7.0
1.037E-03	3.199E-01	ns	B404	0 2 1 1 0	
1.300E-04	4.009E-02	ns	O304	0 0 1 2 2	
2.594E-05	8.000E-03	rt	H302	0 0 2 1 2	intrinsic
1.310E-01	4.040E+01	rt	N056	0 0 1 1 2	average of 2

3993. C₁₉H₂₀N₂O₂

G-21

p,p-Dimethylphenylbutazone

RN: 745-27-7 **MP (°C):**
MW: 308.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.891E-04	1.200E-01	ns	B158	0 0 0 0 1	pH 7.0

3994. C₁₉H₂₀N₂O₃

Oxyphenbutazone

p-Hydroxyphenylbutazone

RN: 129-20-4 **MP (°C):** 124
MW: 324.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.850E-04	6.000E-02	30	D015	2 0 1 1 0	EFG
2.497E-04	8.100E-02	37	D015	2 0 1 1 0	EFG
3.083E-02	1.000E+01	ns	B158	0 0 0 0 1	pH 7.0, <i>sic</i>
>1.54E-03	>5.00E-01	ns	B404	0 2 1 1 0	
6.166E-05	2.000E-02	rt	H302	0 0 2 1 2	intrinsic

3995. C₁₉H₂₀N₄O₆.0.5H₂O6-Methoxy-9-(5-*O*-[4-methylbenzoyl]-β-D-arabinofuranosyl)-9H-purine (hemihydrate)

RN: 121032-20-0 **MP (°C):** 127–128
MW: 409.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.500E-05	1.433E-02	37	M378	1 2 1 1 2	pH 7.2

3996. C₁₉H₂₀N₄O₆2'-(*p*-Tolyllyl)-6-methoxypurine arabinoside

2'-Phenylacetyl-6-methoxypurine arabinoside

RN: 121032-52-8 **MP (°C):** 69–73
MW: 400.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.870E-02	2.350E+01	37	C348	0 0 0 0 0	pH 7.00
5.840E-03	2.338E+00	37	C348	0 0 0 0 0	pH 7.00

3997. C₁₉H₂₀N₄O₆.0.1H₂O9-[5-O-(Benzyl formyl- β -D-arabinofuranosyl)]-6-methoxy-9H-purine (0.1 hydrate)

RN: 121032-36-8 MP (°C): foam

MW: 402.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.050E-02	4.223E+00	37	M378	1 2 1 1 2	pH 7.2

3998. C₁₉H₂₀N₄O₇2'-(*p*-Methoxybenzoyl)-6-methoxypurine arabinoside

RN: 121032-51-7 MP (°C): 71–75

MW: 416.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.660E-03	2.773E+00	37	C348	0 0 0 0 0	pH 7.00

3999. C₁₉H₂₀N₄O₇.0.5H₂O

2'-Phenoxyacetyl-6-methoxypurine arabinoside (hemihydrate)

RN: 145913-46-8 MP (°C): 123–125

MW: 425.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.21E-02	>9.40E+00	37	C348	0 0 0 0 0	pH 7.00

4000. C₁₉H₂₀N₄O₇.0.25H₂O9-[5-O-(4-Methoxybenzoyl- β -D-arabinofuranosyl)]-6-methoxy-9H-purine (0.25 hydrate)

RN: 121032-35-7 MP (°C): 195–197

MW: 420.90 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E-04	8.250E-02	37	M378	1 2 1 1 2	pH 7.2

4001. C₁₉H₂₀N₄O₇.0.05H₂O9-[5-O-(Benzyl acetate- β -D-arabinofuranosyl)]-6-methoxy-9H-purine (0.05 hydrate)

RN: 121032-37-9 MP (°C): 193–195

MW: 417.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.930E-04	1.640E-01	37	M378	1 2 1 1 2	pH 7.2

4002. C₁₉H₂₀O₄

Butylbenzyl phthalate
 Butyl phenyl-methyl phthalate
 Benzylbutyl phthalate
 Phthalate butyl benzyl ester
 Butyl benzyl phthalate
 1,2-Benzenedicarboxylic acid butyl phenylmethyl ester

RN: 85-68-7 **MP (°C):** <35
MW: 312.37 **BP (°C):** 370

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.020E-06	2.818E-03	20	L300	2 1 0 2 2	
3.778E-05	1.180E-02	22	Y419	0 0 0 0 0	
2.273E-06	7.100E-04	24	H116	2 1 0 0 2	
8.644E-06	2.700E-03	25	F067	1 0 2 2 1	

4003. C₁₉H₂₁ClO₄

Isobutyl (+/-)-2-[4-(4-chlorophenoxy)phenoxy]propionate

RN: 51337-71-4 **MP (°C):** 39.5
MW: 348.83 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.160E-04	1.800E-01	22	M161	1 0 0 0 2	

4004. C₁₉H₂₁F₃N₂S

2-Trifluoromethyl-*N,N*-dimethyl-10H-phenothiazine-10-propanamide

RN: 2340-66-1 **MP (°C):**
MW: 366.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-06	1.832E-03	ns	G023	0 0 1 1 0	

4005. C₁₉H₂₁NO

Doxepin
 Adapin
 Deptran
 Sinequan

RN: 1668-19-5 **MP (°C):** 120
MW: 279.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-04	3.157E-02	25	E051	1 0 2 1 2	

4006. C₁₉H₂₁NO₃

Thebaine

Paramorphine

Morphinan, 6,7,8,14-tetrahydro-4,5 α -epoxy-3,6-dimethoxy-17-methyl-**RN:** 115-37-7 **MP (°C):****MW:** 311.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-03	6.850E-01	15	K059	2 2 2 0 1	

4007. C₁₉H₂₁N₃O

Zolpidem

RN: 82626-48-0 **MP (°C):****MW:** 307.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.25E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4008. C₁₉H₂₁N₅O₂

Dis. A. 6

Propanenitrile, 3-[butyl[4-[(4-nitrophenyl)azo]phenyl]amino]-

RN: 69472-19-1 **MP (°C):** 118**MW:** 351.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-08	7.028E-06	25	B333	0 0 0 0 0	

4009. C₁₉H₂₁N₅O₂

Dye VII

4-[[4-(*N*-Butyl-*N*-ethylnitrite)amino)phenyl]azo]nitrobenzene**RN:** **MP (°C):****MW:** 351.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-07	1.687E-04	71.80	B198	1 2 1 1 1	
9.700E-07	3.409E-04	84.10	B198	1 2 1 1 1	
2.020E-06	7.099E-04	97.40	B198	1 2 1 1 2	

4010. C₁₉H₂₁N₅O₄

Prazosin

Minipress

Pressin

RN: 19216-56-9 **MP (°C):**
MW: 383.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.346E-06	3.200E-03	22.5	B422	0 0 0 0 0	

4011. C₁₉H₂₁N₅O₅

9-[5'-(O-Hydrocinnamoyl)-β-D-arabinofuranosyl]adenine ester

RN: 68325-41-7 **MP (°C):**
MW: 399.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.756E-03	1.500E+00	ns	B134	0 1 1 1 1	

4012. C₁₉H₂₂Cl₂O₂1-Methyl-1,1-dichloro-2,2-bis(*p*-ethoxyphenyl)ethane

RN: 56265-23-7 **MP (°C):**
MW: 353.29 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.415E-07	5.000E-05	rt	C122	0 0 0 0 0	

4013. C₁₉H₂₂N₂O

Cinchonidine

Cinchonidin

(8α,9R)-Cinchonan-9-ol

L-Cinchonidine

RN: 485-71-2 **MP (°C):** 210
MW: 294.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.650E-01	15	K059	2 2 2 0 0	
9.511E-05	2.800E-02	22	M459	0 0 0 0 0	
6.793E-04	2.000E-01	25	F300	1 0 0 0 0	
1.970E-03	5.800E-01	100	F300	1 0 0 0 1	
6.792E-04	2.000E-01	c	D004	0 0 0 0 0	
8.490E-04	2.499E-01	rt	D021	0 0 1 1 1	

4014. C₁₉H₂₂N₂O

Cinchonine
 Cinchonan-9-ol
 (+)-Cinchonine
 (9S)-Cinchonan-9-ol

RN: 118-10-5 **MP (°C):** 265
MW: 294.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-06	1.413E-03	15	K059	2 2 2 0 1	
2.378E-05	7.000E-03	22	M459	0 0 0 0 0	
9.253E-04	2.724E-01	25	D004	0 0 0 0 0	
9.171E-04	2.700E-01	100	F300	1 0 0 0 1	
8.150E-04	2.399E-01	rt	D021	0 0 1 1 1	

4015. C₁₉H₂₂N₂OS

Acetylpromazine
 3-Acetyl-10-(3-dimethylaminopropyl)phenothiazine
 Plegicil
 Vetranquil
 Notensil
 Plivafen

RN: 61-00-7 **MP (°C):**
MW: 326.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.901E-05	1.600E-02	25	L045	1 1 1 1 2	intrinsic

4016. C₁₉H₂₂N₂O₅

2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester
 Naproxen N-methyl-N-carbamoyl methyl glycolamide ester
RN: 114681-69-5 **MP (°C):** 179
MW: 358.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.646E-04	5.900E-02	21	B331	0 0 0 0 0	

4017. C₁₉H₂₂N₂S

Mepazine
 Pecazine
RN: 60-89-9 **MP (°C):** 80
MW: 310.46 **BP (°C):** 233

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-05	5.588E-03	24	G022	2 0 1 1 1	

4018. C₁₉H₂₃ClO₂1-Chloro-1-methyl-2,2-bis(*p*-ethoxylphenyl)ethane

RN: 56265-22-6 MP (°C):

MW: 318.85 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.760E-06	8.800E-04	rt	C122	0 0 0 0 0	

4019. C₁₉H₂₃NO₃

Ethylmorphine

7,8-Didehydro-4,5-epoxy-3-ethoxy-17-methylmorphinan-6-ol

RN: 76-58-4 MP (°C):

MW: 313.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.916E-03	2.794E+00	20	K052	1 1 1 1 2	

4020. C₁₉H₂₃NO₄1-Methyl-1-nitro-2,2-bis(*p*-ethoxylphenyl)ethane

RN: 26258-70-8 MP (°C):

MW: 329.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.093E-06	3.600E-04	rt	C122	0 0 0 0 0	

4021. C₁₉H₂₃NO₅2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-[(2-hydroxyethyl)methylamino]-2-oxoethyl esterNaproxen *N*-methyl-*N*-ethanol glycolamide ester

RN: 114665-19-9 MP (°C): 110

MW: 345.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.053E-04	1.400E-01	21	B331	0 0 0 0 0	

4022. C₁₉H₂₃N₃

Amitraz

1,5-Di(2,4-dimethylphenyl)-3-methyl-1,3,5-triazapenta-1,4-diene

Ovasyn

Mitac

Triazid

Baam

RN: 33089-61-1 **MP (°C):** 86.5**MW:** 293.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.408E-06	1.000E-03	rt	M161	0 0 0 0 0	

4023. C₁₉H₂₃N₃O₂

Ergonovine

9,10-Didehydro-N-(2-hydroxy-1-methylethyl)-6-methylergoline-8-carboxamide

Ergometrine

RN: 60-79-7 **MP (°C):****MW:** 325.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.21E+00	>3.94E+02	25	B443	0 0 0 0 0	

4024. C₁₉H₂₃N₅O₄

Benzoic acid, 4-[(dimethylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c]pyridin-1-yl)methoxy]ethyl ester

1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.

RN: 137605-68-6 **MP (°C):****MW:** 385.43 **BP (°C):** 651.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.373E-03	1.300E+00	21	B419	1 1 2 2 1	int

4025. C₁₉H₂₄N₂

1-(Diphenylmethyl)-4-ethylpiperazine

RN: **MP (°C):****MW:** 280.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.030E-03	5.693E-01	25	M438	0 0 0 0 0	

4026. C₁₉H₂₄N₂

Imipramine

10,11-Dihydro-*N,N*-dimethyl-5H-dibenz[b,f]azepine-5-propanamine

5-[3-(Dimethylamino)propyl]-10,11-dihydro-5H-dibenz[b,f]azepine

RN: 50-49-7 MP (°C): 174

MW: 280.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.500E-05	1.823E-02	24	G022	2 0 1 1 1	

4027. C₁₉H₂₄N₂O

Hydrocinchonine

Hydrocinchonin

Cinchotine

RN: 485-65-4 MP (°C): 268

MW: 296.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.362E-03	7.000E-01	16	F300	1 0 0 0 1	
2.593E-03	7.686E-01	25	D004	0 0 0 0 0	

4028. C₁₉H₂₄N₂OS

Methotriimeprazine

Levomepromazine

RN: 60-99-1 MP (°C): 117

MW: 328.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.089E-05	2.000E-02	25	A081	1 0 1 1 0	EFG

4029. C₁₉H₂₄N₂O₂

Praziquantel

2-Cyclohexyl-carbonyl-1,3,4,6,7,11b-hexahydro-2H-pyrazine(2,1-a)isoquinoline-4-one

Biltricide

Droncit

RN: 55268-74-1 MP (°C):

MW: 312.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.000E-04	2.812E-01	30	B402	2 0 1 1 0	EFG
1.280E-03	4.000E-01	ns	K444	0 0 0 0 0	

4030. C₁₉H₂₄N₂O₂S

Cyclohexyl-*p*-toluene sulfonamide
Cyclohexyl-4-toluene sulfonamide

RN: **MP (°C):**
MW: 344.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.742E-04	6.000E-02	ns	F014	0 0 0 0 0	

4031. C₁₉H₂₄N₄O₇

Propyloxycarbonyl-mitomycin C

RN: **MP (°C):**
MW: 420.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.300E-04	1.387E-01	25	M316	1 1 1 1 2	

4032. C₁₉H₂₄O

1,1-Dimethyl-2-(*p*-methylphenyl)-2-*p*-ethoxylphenyl)ethane

RN: 56265-26-0 **MP (°C):**
MW: 268.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.706E-07	1.800E-04	rt	C122	0 0 0 0 0	

4033. C₁₉H₂₄O₂

1,1,1-Trimethyl-2,2-bis(*p*-methyloxylphenyl)ethane

RN: 4741-74-6 **MP (°C):**
MW: 284.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.426E-06	6.900E-04	rt	C122	0 0 0 0 0	

4034. C₁₉H₂₄O₃

Adrenosterone

Androstene-3,11,17-trione

RN: 382-45-6 **MP (°C):** 220
MW: 300.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.279E-04	9.849E-02	23.5	J003	2 0 2 1 2	average of 2
2.610E-04	7.840E-02	37	H004	0 0 0 0 0	
5.059E-04	1.520E-01	37	J003	1 0 2 1 2	

4035. C₁₉H₂₅NO*N,N*-Dicyclopentylcinnamamide2-Propenamide, *N,N*-dicyclopentyl-3-phenyl-

RN: 59832-08-5 MP (°C):

MW: 283.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.750E-07	2.196E-04	ns	H350	0 0 0 0 0	

4036. C₁₉H₂₆I₃N₃O₁₀1,3-Benzenedicarboxamide, *N,N'*-bis[2-hydroxy-1,1-bis(hydroxymethyl)ethyl]-5-[(2-hydroxy-1-oxopropyl)amino]-2,4,6-triido-, (*S*)-

RN: 77868-46-3 MP (°C):

MW: 837.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.342E-02	1.961E+01	25	P091	0 0 0 0 0	

4037. C₁₉H₂₆N₆O₄SBenzenesulfonamide, 4-(1,3-diethyl-2,3,6,7-tetrahydro-2,6-dioxo-1H-purin-8-yl)-*N*-[2-(dimethylamino)ethyl]-

RN: 89073-49-4 MP (°C): 264

MW: 434.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.532E-04	1.100E-01	ns	H316	0 0 0 0 0	pH 7.4
2.647E-02	1.150E+01	ns	H316	0 0 0 0 0	0.1N HCL

4038. C₁₉H₂₆O

δ-4-Androstene-3-one

RN: MP (°C):

MW: 270.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-06	<2.70E-04	25	E014	2 2 2 1 0	pH 7.3

4039. C₁₉H₂₆O₂

Androstenedione

4-Androstene-3,17-dione

Androst-4-en-3,17-dion

RN: 63-05-8 **MP (°C):**
MW: 286.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-04	5.728E-02	25	E014	2 2 2 1 2	pH 7.3
2.840E-02	8.133E+00	25	P324	0 0 0 0 0	
1.399E-04	4.007E-02	37	H034	1 0 2 1 2	pH 7.4
1.700E-04	4.870E-02	37	L010	2 0 2 1 1	

4040. C₁₉H₂₇N₃O

Doxylamine ethanamine

RN: **MP (°C):**
MW: 313.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-02	9.403E+00	37.5	L034	2 2 0 1 2	pH 7.4

4041. C₁₉H₂₇N₃O₂2-Propoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide*N*-[2-(Diethylamino)ethyl]-2-propoxyquinoline-4-carboxamide

RN: 2717-00-2 **MP (°C):**
MW: 329.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.980E-04	1.311E-01	ns	B018	0 0 0 0 2	
3.980E-04	1.311E-01	ns	M066	0 0 0 0 2	

4042. C₁₉H₂₈Cl₂O₃2,4-Dichlorophenoxyacetic acid *n*-undecyl ester

RN: 65267-95-0 **MP (°C):**
MW: 375.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.977E-05	7.420E-03	ns	M120	0 0 1 1 2	

4043. C₁₉H₂₈N₄O₆

2'-Octanyl-6-methoxypurine arabinoside

RN: 145913-41-3 MP (°C): 75-77

MW: 408.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.110E-04	2.496E-01	37	C348	0 0 0 0 0	pH 7.00

4044. C₁₉H₂₈O

7α-Methyl-19-nortestosterone

Trestolone

19-Nor-7α-methyltestosterone

RN: 3764-87-2 MP (°C):

MW: 272.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.377E-04	9.200E-02	37	H004	0 0 0 0 0	

4045. C₁₉H₂₈O₂

Androstanedione

5α-Androstane-3,17-dione

RN: 846-46-8 MP (°C): 142

MW: 288.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.141E-04	3.290E-02	23.5	J003	1 0 2 1 2	average of 2
2.200E-04	6.346E-02	25	E014	2 2 2 1 2	pH 7.3
1.685E-04	4.860E-02	37	J003	1 0 2 1 2	average of 2

4046. C₁₉H₂₈O₂

Testosterone

17β-Hydroxyandrost-4-en-3-one

Halotensin

Virilon

Oreton

Testex

RN: 58-22-0 MP (°C): 155

MW: 288.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.600E-05	1.615E-02	10	B012	2 0 1 1 0	
6.390E-05	1.843E-02	10	L017	2 2 2 2 2	
2.254E-04	6.500E-02	15	F042	2 2 2 2 1	
7.550E-05	2.178E-02	15	L017	2 2 2 2 2	
7.900E-05	2.279E-02	20	B012	2 0 1 1 0	

(continued)

4046. C₁₉H₂₈O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.430E-04	7.009E-02	20	F012	1 0 1 1 1	
2.392E-04	6.900E-02	20	F042	2 2 2 2 1	
8.460E-05	2.440E-02	20	G072	1 2 2 1 2	
7.790E-05	2.247E-02	20	L017	2 2 2 2 2	
8.000E-05	2.307E-02	20	L070	1 2 0 2 0	EFG
6.870E-05	1.982E-02	20	L077	1 2 2 2 2	
8.000E-04	2.307E-01	20	L087	1 1 2 1 0	EFG
6.240E-05	1.800E-02	22.5	B422	2 0 2 2 2	
8.100E-05	2.336E-02	25	B012	2 0 1 1 0	
9.500E-05	2.740E-02	25	B041	1 0 2 2 1	
2.531E-04	7.300E-02	25	F042	2 2 2 2 1	
8.321E-05	2.400E-02	25	K003	2 1 1 1 1	
1.664E-04	4.800E-02	25	L009	1 0 0 1 1	
8.480E-05	2.446E-02	25	L017	2 2 2 2 2	
6.934E-05	2.000E-02	25	L338	1 0 1 1 2	
1.040E-04	3.000E-02	27.34	L077	1 2 2 2 2	
1.060E-04	3.057E-02	30	B012	2 0 1 1 0	
2.670E-04	7.700E-02	30	F042	2 2 2 2 1	
9.790E-05	2.824E-02	30	L017	2 2 2 2 2	
1.100E-04	3.173E-02	30	L068	1 0 0 1 0	EFG
2.500E-04	7.211E-02	30	L344	2 0 1 1 0	
1.040E-04	3.000E-02	30	M007	2 2 1 2 2	average of 8
8.876E-05	2.560E-02	30	T005	2 0 2 2 2	
1.096E-04	3.163E-02	31	A025	2 2 2 2 0	EFG
1.300E-04	3.750E-02	35	L017	2 2 2 2 2	
1.397E-04	4.029E-02	35	L077	1 2 2 2 2	
1.950E-04	5.624E-02	37	B013	1 0 2 2 0	average
1.250E-04	3.605E-02	37	E014	2 2 2 1 2	pH 7.3
1.013E-04	2.922E-02	37	H034	1 0 2 1 2	pH 7.4
1.259E-04	3.631E-02	37.50	B041	1 0 2 2 0	EFG
1.260E-04	3.634E-02	37.50	B041	1 0 2 2 2	
1.400E-04	4.038E-02	40	B012	2 0 1 1 0	
1.570E-04	4.528E-02	40	L017	2 2 2 2 2	
3.000E-04	8.653E-02	40	L070	1 2 0 2 0	EFG
1.702E-04	4.909E-02	42.34	L077	1 2 2 2 2	
1.870E-04	5.394E-02	45	L017	2 2 2 2 2	
2.100E-04	6.057E-02	50	B012	2 0 1 1 0	
2.350E-04	6.778E-02	50	L017	2 2 2 2 2	
2.053E-04	5.922E-02	50	L077	1 2 2 2 2	
6.795E-05	1.960E-02	ns	B057	0 2 1 1 2	
3.814E-05	1.100E-02	ns	B338	0 0 0 0 1	

4047. C₁₉H₂₈O₂

5,6-Dehydroisoandrosterone

Prasterone

Dehydroepiandrosterone

Dehydroisoandrosterone

RN: 53-43-0**MP (°C):** 140.5**MW:** 288.43**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.558E-05	2.180E-02	23.5	J003	2 0 2 1 2	average of 6
1.000E-04	2.884E-02	37	E014	2 2 2 1 2	pH 7.3
1.040E-04	3.000E-02	37	H034	1 0 2 1 2	pH 7.4
1.144E-04	3.300E-02	37	J003	1 0 2 1 2	average of 4
8.633E-05	2.490E-02	ns	B057	0 2 1 1 2	

4048. C₁₉H₂₈O₂.H₂O

Testosterone (monohydrate)

Testosterone monohydrate -I

RN: 58-22-0**MP (°C):****MW:** 306.45**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.265E-05	1.920E-02	15	F042	2 2 2 2 2	crystal-II
5.352E-05	1.640E-02	15	F042	2 2 2 2 2	crystal-I
7.081E-05	2.170E-02	20	F042	2 2 2 2 2	crystal-II
6.265E-05	1.920E-02	20	F042	2 2 2 2 2	crystal-I
8.256E-05	2.530E-02	25	F042	2 2 2 2 2	crystal-II
7.310E-05	2.240E-02	25	F042	2 2 2 2 2	crystal-I
9.333E-05	2.860E-02	30	F042	2 2 2 2 2	crystal-II
8.484E-05	2.600E-02	30	F042	2 2 2 2 2	crystal-I

4049. C₁₉H₂₈O₃

11-Ketoetiocholanolone

3 α -Hydroxy-5 β -androstane-11,17-dione

Etiocholanol-11-one

Ba 2684

RN: 739-27-5**MP (°C):****MW:** 304.43**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.455E-04	2.269E-01	23	J003	2 0 2 1 2	average of 4
9.457E-04	2.879E-01	37	J003	1 0 2 1 2	average of 2

4050. C₁₉H₂₉ClN₅O₆

Terazosin

Hytrin

1-(4-Amino-6,7-dimethoxy-2-quinazolinyl)-4-((tetra-hydro-2-furanyl)carbonyl)-, monohydrochloride, dihydrate

(RS)-Piperazine

RN: 63590-64-7 **MP (°C):**
MW: 458.93 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.669E-05	3.060E-02	22.5	B440	0 0 0 0 0	

4051. C₁₉H₂₉NO*n*-Decylcinnamamide2-Propenamide, *N*-decyl-3-phenyl-

RN: 59832-02-9 **MP (°C):**
MW: 287.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.530E-06	7.272E-04	ns	H350	0 0 0 0 0	

4052. C₁₉H₂₉NO

Procyclidine

Kemadrin

RN: 77-37-2 **MP (°C):**
MW: 287.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.669E-06	1.055E-03	22.5	B440	0 0 0 0 0	

4053. C₁₉H₂₉N₅O₆

9-(1,3-Dipivaloate-2-propoxymethyl)guanine

RN: 88110-72-9 **MP (°C):** 231
MW: 423.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.653E-05	7.000E-03	25	B360	0 0 0 0 0	

4054. C₁₉H₃₀O

Androstane-17-one

RN: 36378-49-1 **MP (°C):** 119
MW: 274.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.00E-07	<5.49E-05	25	E014	2 2 2 1 0	pH 7.3

4055. C₁₉H₃₀OS

Epitiostanol

RN: 2363-58-8 **MP (°C):** 127
MW: 306.51 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.915E-06	1.200E-03	37	H120	1 1 1 1 1	normal saline

4056. C₁₉H₃₀O₂

Epiandrosterone

Isoandrosterone

RN: 481-29-8 **MP (°C):** 161
MW: 290.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.955E-05	2.020E-02	23.5	J003	2 0 2 1 2	average of 5
8.160E-05	2.370E-02	37	J003	1 0 2 1 2	average of 3

4057. C₁₉H₃₀O₂

Androsterone

3 α -Hydroxy-17-androstanone3 α -Hydroxy-5 α -androstan-17-oneHydroxy-5 α -androstan-17-one

Epihydroxyetioallocholan-17-one

Hydroxy-17-androstanone

RN: 53-41-8 **MP (°C):** 185
MW: 290.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-05	1.150E-02	23.5	J003	2 0 2 1 2	average of 2
4.300E-05	1.249E-02	37	E014	2 2 2 1 1	pH 7.3
6.163E-05	1.790E-02	37	J003	1 0 2 1 2	average of 2

4058. C₁₉H₃₀O₂

Stanolone

Androstanolone

RN: 521-18-6 **MP (°C):** 181.0
MW: 290.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.185E+00	3.443E+02	ns	B057	0 2 1 1 2	

4059. C₁₉H₃₀O₂

Etiocholanolone

3 α -Hydroxy-5 β -androstane-17-one

5-Isoandrosterone

RN: 53-42-9 **MP (°C):**
MW: 290.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.002E-04	2.910E-02	23.5	J003	2 0 2 1 2	average of 2
7.000E-05	2.033E-02	25	E014	2 2 2 1 1	pH 7.3, pyrogen

4060. C₁₉H₃₀O₃*p*-(Dodecyloxy)benzoic acidDodecyl *p*-hydroxybenzoate

RN: 2312-15-4 **MP (°C):** 95
MW: 306.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.569E-03	1.094E+00	25	D081	1 2 2 1 2	

4061. C₁₉H₃₀O₃Androstane-3 β ,11 β -diol-17-one

Hydroxyisoandrosterone

RN: 514-17-0 **MP (°C):** 235
MW: 306.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.552E-04	7.819E-02	23.5	J003	1 0 2 1 2	average of 2

4062. C₁₉H₃₀O₃

11-Hydroxyetiocholanolone

5β-Androstan-17-one, 3α,11-dihydroxy-

RN: 3272-49-9 **MP (°C):****MW:** 306.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	4.290E-02	23.5	J003	2 0 1 1 2	average of 2

4063. C₁₉H₃₁NO₂Dodecyl *p*-aminobenzoate*p*-Aminobenzoic acid dodecyl ester**RN:** 20043-94-1 **MP (°C):****MW:** 305.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-08	4.887E-06	37	F006	1 1 2 2 1	

4064. C₁₉H₃₁NO₃

4-Hexoxybenzoic acid-2-(diethyl-amino)ethyl ester

RN: 38973-74-9 **MP (°C):****MW:** 321.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.286E-02	ns	M066	0 0 0 0 1	

4065. C₁₉H₃₁NO₉

Metoprolol tartrate

1-(Isopropylamino)-3-(*p*-(2-methoxyethyl)phenoxy)-2-propanol (2:1)**RN:** 56392-17-7 **MP (°C):****MW:** 417.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-01	4.300E+01	25	A412	1 0 2 2 1	int

4066. C₁₉H₃₂

2-Phenyltridecane

RN: **MP (°C):****MW:** 260.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4067. C₁₉H₃₂

6-Phenyltridecane

RN:**MW:** 260.47**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4068. C₁₉H₃₂

5-Phenyltridecane

RN:**MW:** 260.47**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4069. C₁₉H₃₂

4-Phenyltridecane

RN:**MW:** 260.47**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4070. C₁₉H₃₂

3-Phenyltridecane

RN:**MW:** 260.47**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.042E-06	25	S377	0 0 0 0 0	

4071. C₁₉H₃₂N₂O₂

4-Hexylaminobenzoic acid-2-(diethyl-amino)ethyl ester

RN: 16488-57-6**MP (°C):****MW:** 320.48**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-04	6.089E-02	ns	M066	0 0 0 0 1	

4072. C₁₉H₃₂O₃

4-Nonylphenol diethoxylate

RN: 20427-84-3 **MP (°C):**
MW: 308.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.180E-05	3.640E-03	2	A335	0 0 0 0 0	
1.080E-05	3.331E-03	10	A335	0 0 0 0 0	
1.096E-05	3.380E-03	10	A335	0 0 0 0 0	
9.700E-06	2.992E-03	14	A335	0 0 0 0 0	
9.726E-06	3.000E-03	14	A335	0 0 0 0 0	
1.100E-05	3.393E-03	20.5	A335	0 0 0 0 0	
1.096E-05	3.380E-03	20.5	A335	0 0 0 0 0	
1.200E-05	3.702E-03	25	A335	0 0 0 0 0	
1.196E-05	3.690E-03	25	A335	0 0 0 0 0	

4073. C₁₉H₃₄O₃

Methoprene

Isopropyl (2E,4E)-11-methoxy-3,7,11-trimethyl-2,4-dodecadienoate

Kabat

Precor

Dianex

Pharorid

RN: 40596-69-8 **MP (°C):** 164
MW: 310.48 **BP (°C):** 100

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.477E-06	1.390E-03	25	D302	1 0 0 0 2	
6.442E-06	2.000E-03	ns	M110	0 0 0 0 0	EFG

4074. C₁₉H₄₀

2,6,10,14-Tetramethylpentadecane

Pristane

RN: 1921-70-6 **MP (°C):**
MW: 268.53 **BP (°C):** 296

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.724E-11	1.000E-08	25	T423	0 0 0 0 0	

4075. C₂₀H₉Cl₃F₅N₃O₃

Chlorfluazuron

Atabron

Benzamide, *N*-[4-(3-chloro-5-trifluoromethyl-2-pyridinyl-oxy)-3,5-dichloro-phenyl-aminocarbonyl]-2,6-difluoro

Jupiter

RN: 71422-67-8 **MP (°C):**
MW: 540.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.219E-09	1.200E-06	20	M402	0 0 0 0 0	

4076. C₂₀H₁₂

Benzo(a)pyrene

1,2-Benzopyrene

3,4-Benzpyrene

Benzo[a]pyrene

Benz[a]pyrene

RN: 50-32-8 **MP (°C):** 179
MW: 252.32 **BP (°C):** 310

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.309E-09	8.350E-07	15	B385	0 0 0 0 0	
2.000E-09	5.046E-07	20	E009	1 0 0 0 1	
2.972E-05	7.500E-03	23	T025	1 2 0 1 1	
6.341E-09	1.600E-06	25	B319	2 0 1 2 1	
5.667E-09	1.430E-06	25	B385	0 0 0 0 0	
7.213E-09	1.820E-06	25	D406	1 2 2 2 2	
4.400E-10	1.110E-07	25	K123	1 0 2 2 1	
1.506E-08	3.800E-06	25	L332	1 1 1 1 2	
1.506E-08	3.800E-06	25	M064	1 1 2 2 1	
1.500E-08	3.785E-06	25	M342	1 0 1 1 1	
6.428E-09	1.622E-06	25.04	M183	1 2 1 1 2	
1.585E-08	4.000E-06	27	D003	1 0 0 1 1	
9.083E-09	2.292E-06	30.04	M183	1 2 1 1 2	
1.098E-08	2.770E-06	35	B385	0 0 0 0 0	
1.506E-08	3.800E-06	ns	M344	0 0 0 0 2	
2.400E-08	6.056E-06	ns	W005	0 0 1 2 1	
4.756E-09	1.200E-06	ns	W302	0 0 0 0 1	

4077. C₂₀H₁₂

Benzo(k)fluoranthene

11,12-Benzo[k]fluoranthene

11,12-Benzofluoranthene

8,9-Benzofluoranthene

2,3,1',8'-Binaphthylene

B[K]F

RN: 207-08-9 MP (°C): 216

MW: 252.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.320E-09	1.090E-06	25	D406	1 2 2 2 2	
3.171E-09	8.000E-07	ns	W302	0 0 0 0 0	

4078. C₂₀H₁₂

Benzo(j)fluoranthene

Benzo[l]fluoranthene

Benzo-12,13-fluoranthene

10,11-Benzofluoranthene

RN: 205-82-3 MP (°C): 165

MW: 252.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.908E-09	2.500E-06	ns	W302	0 0 0 0 1	

4079. C₂₀H₁₂

Benzo(e)pyrene

4,5-Benzopyrene

B[E]P

RN: 192-97-2 MP (°C): 178.5

MW: 252.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-09	9.840E-07	25	K123	1 0 2 2 1	
~1.59E-08	~4.00E-06	25	S227	1 2 1 1 0	
6.625E-02	1.672E+01	318	S355	1 1 1 2 0	EFG
1.192E-01	3.007E+01	330	S355	1 1 1 2 0	EFG
1.524E-01	3.846E+01	335	S355	1 1 1 2 0	EFG
2.066E-01	5.213E+01	342	S355	1 1 1 2 0	EFG
4.246E-01	1.071E+02	361	S355	1 1 1 2 0	EFG
4.559E-01	1.150E+02	365	S355	1 1 1 2 0	EFG

4080. C₂₀H₁₂

Perylene

Dibenz[de,kl]anthracene

peri-Dinaphthalene

RN: 198-55-0

MP (°C): 273

MW: 252.32

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-10	1.060E-07	20	E009	1 0 0 1 1	
1.585E-09	4.000E-07	25	M064	1 1 2 2 0	
1.600E-09	4.037E-07	25	M342	1 0 1 1 1	
<1.98E-09	<5.00E-07	27	D003	1 0 0 1 0	
1.585E-09	4.000E-07	ns	M344	0 0 0 0 1	

4081. C₂₀H₁₂

Benzo(b)fluoranthene

3,4-Benzofluoranthene

2,3-Benzofluoranthene

B[B]F

RN: 205-99-2

MP (°C): 108

MW: 252.32

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.945E-09	1.500E-06	ns	W302	0 0 0 0 1	

4082. C₂₀H₁₃N

13H-Dibenzo(a,i)carbazole

1:2,7:8-Dibenzocarbazole

RN: 239-64-5

MP (°C): 220

MW: 267.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.00E-08	<1.34E-05	22	B175	1 0 1 1 0	<i>sic</i>
3.890E-08	1.040E-05	24	H106	1 0 2 2 2	
3.890E-08	1.040E-05	24	M303	1 0 1 1 2	

4083. C₂₀H₁₃N

3,4,5,6-Dibenzocarbazole

3:4,5:6-Dibenzocarbazole

RN: 194-59-2

MP (°C): 158

MW: 267.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-07	5.347E-05	22	B175	1 0 1 1 0	

4084. C₂₀H₁₃N

1,2,5,6-Dibenzocarbazole

1:2,5:6-Dibenzocarbazole

RN: 207-84-1 **MP (°C):**
MW: 267.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.337E-05	22	B175	1 0 1 1 0	

4085. C₂₀H₁₄

3,4'-Ace-1,2-benzanthracene

Benz[k]acephenanthrene

RN: 5779-79-3 **MP (°C):**
MW: 254.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-08	2.700E-06	27	D003	1 0 0 1 1	

4086. C₂₀H₁₄

Cholanthrene

1,2-Dihydroxybenz[j]aceanthrylene

RN: 479-23-2 **MP (°C):** 173
MW: 254.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.376E-08	3.500E-06	27	D003	1 0 0 1 1	

4087. C₂₀H₁₄I₆N₂O₆

Di(3-carboxy-2,4,6-triiodoanilido)adipic acid

Iodipamide

RN: 606-17-7 **MP (°C):** 306
MW: 1139.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.036E-04	4.600E-01	20	N035	1 1 2 1 1	
>4.38E-04	>5.00E-01	ns	B404	0 2 1 1 0	
1.404E-04	1.600E-01	ns	H055	0 0 0 0 0	

4088. C₂₀H₁₄N₂O₂

Disperse blue 19

C.I. Disperse blue 19

RN: 4395-65-7

MP (°C): 194

MW: 314.35

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.100E-10	1.918E-07	25	B333	0 0 0 0 0	
2.100E-07	6.601E-05	60.0	D093	1 2 1 2 0	EFG
5.000E-07	1.572E-04	71.8	D093	1 2 1 2 0	EFG
1.700E-06	5.344E-04	81.4	D093	1 2 1 2 0	EFG
4.200E-06	1.320E-03	97.4	D093	1 2 1 2 0	EFG

4089. C₂₀H₁₄O₂

3,3-Diphenylphthalide

3,3-Diphenyl-phthalid

RN: 596-29-2

MP (°C):

MW: 286.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-04	4.000E-02	25	F300	1 0 0 0 0	

4090. C₂₀H₁₄O₄

Phenolphthalein

2-[bis(4-Hydroxyphenyl)methyl]benzoic acid

Espotabs

Alophen

Figsen

Laxlettes

RN: 77-09-8

MP (°C): 260.0

MW: 318.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.283E-06	2.000E-03	25	H064	1 2 2 0 2	
7.476E-04	2.380E-01	100	H064	1 2 2 0 2	
1.256E-03	3.998E-01	rt	D021	0 0 1 1 0	

4091. C₂₀H₁₄O₄

Phenyl phthalate

Diphenyl phthalate

RN: 84-62-8

MP (°C): 71

MW: 318.33

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.576E-07	8.200E-05	24	H116	2 1 0 0 1	

4092. C₂₀H₁₄O₄Diphenyl *o*-phthalate

RN: **MP (°C):** 72 C
MW: 318.33 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.424E-06	3.000E-03	25	S417	0 0 0 0 0	

4093. C₂₀H₁₅O₅P

bis(4-Carboxyphenyl)phenylphosphine oxide

BCPPO

RN: 803-19-0 **MP (°C):**
MW: 366.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
2.000E-04	7.326E-02	23	W402	0 0 0 0 0	
3.166E-04	1.160E-01	32	W402	0 0 0 0 0	
4.666E-04	1.709E-01	40	W402	0 0 0 0 0	
6.943E-04	2.543E-01	50	W402	0 0 0 0 0	
1.011E-03	3.702E-01	60	W402	0 0 0 0 0	
1.638E-03	6.000E-01	70	W402	0 0 0 0 0	
1.987E-03	7.280E-01	75	W402	0 0 0 0 0	

4094. C₂₀H₁₆

5,6-Dimethylchrysene

Chrysene, 5,6-dimethyl-

RN: 3697-27-6 **MP (°C):** 127
MW: 256.35 **BP (°C):** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
9.752E-08	2.500E-05	27	D003	1 0 0 1 1	

4095. C₂₀H₁₆

9,10-Dimethyl-1,2-benzanthracene

7,12-Dimethyl-1,2-benzanthracene

7,12-Dimethylbenz[a]anthracene

9,10-Dimethyl-benz[a]anthracene

RN: 56-56-4 **MP (°C):** 122
MW: 256.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref	Evaluation (T P E A A)	Comments
9.518E-08	2.440E-05	24	H106	1 0 2 2 2	
2.145E-07	5.500E-05	24	H116	2 1 0 0 1	
9.752E-08	2.500E-05	24	M129	1 2 1 1 1	
2.380E-07	6.100E-05	25	M064	1 1 2 2 1	
9.518E-08	2.440E-05	25	M156	1 2 1 1 2	
1.677E-07	4.300E-05	27	D003	1 0 0 1 1	

4096. C₂₀H₁₆

10-Ethyl-1,2-benzanthracene

10-Ethylbenz[a]anthracene

RN: 14854-08-1 **MP (°C):** 114
MW: 256.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.755E-07	4.500E-05	27	D003	1 0 0 1 1	
1.560E-07	4.000E-05	27	D043	2 0 0 0 0	average of 2

4097. C₂₀H₁₆O₄

Phenolphthalin

Benzoic acid, 2-[bis(4-hydroxyphenyl)methyl]-

RN: 81-90-3 **MP (°C):** 237
MW: 320.35 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.463E-04	1.750E-01	20	F300	1 0 0 0 2	

4098. C₂₀H₁₇FO₃S

Sulindac

Aclin

Clinoril

Clusinol

Saldac

RN: 38194-50-2 **MP (°C):**
MW: 356.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.964E-05	7.000E-03	37	Y421	0 0 0 0 0	

4099. C₂₀H₁₈O₂Sn

Triphenyltin hydroxide acetate

Fentin acetate

RN: 900-95-8 **MP (°C):** 120
MW: 409.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.845E-05	2.800E-02	20	M161	1 0 0 0 1	

4100. C₂₀H₁₈O₁₀

Biphenyl dimethyl dicarboxylate

DDB

RN: **MP (°C):**
MW: 418.36 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.004E-05	4.200E-03	ns	K446	0 0 0 0 0	

4101. C₂₀H₁₉NO₃

Acronine

3,12-Dihydro-6-methoxy-3,3,12-trimethyl-7H-pyrano(2,3-c)acridin-7-one

Acronycine

RN: 7008-42-6 **MP (°C):** 175–176
MW: 321.38 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.779E-06	2.500E-03	22	B064	1 0 1 1 0	
8.401E-06	2.700E-03	25	R071	0 0 0 0 0	

4102. C₂₀H₁₉NO₅.6H₂O

Berberine (hexahydrate)

Berberine

RN: 2086-83-1 **MP (°C):** 145dec
MW: 461.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.422E-02	4.348E+01	25	D004	0 0 0 0 0	

4103. C₂₀H₁₉N₃

Rosaniline

Basic violet 14

C.I. 42510

Calcozine magenta xx

Cerise B

RN: 632-99-5 **MP (°C):**
MW: 301.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.951E-04	2.999E-01	rt	D021	0 0 1 1 0	

4104. C₂₀H₁₉N₃O₅

1H-Benzimidazole-1-carboxylic acid, 6-benzoyl-2-[(methoxycarbonyl)amino]-, propyl ester

RN: 153474-31-8 MP (°C): 113.5

MW: 381.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.311E-05	5.000E-03	21	N337	0 0 0 0 0	pH 5
1.311E-05	5.000E-03	21	N337	0 0 0 0 0	pH 5

4105. C₂₀H₂₀ClNO₇

BTA-243

1,3-Benzodioxole-2,2-dicarboxylic acid, 5-[2-[[2-(3-chlorophenyl)-2-hydroxyethyl]amino]propyl]-

RN: MP (°C):
MW: 421.84 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.890E-03	3.750E+00	25	B421	0 0 1 1 0	Zwitterion, EFG

4106. C₂₀H₂₀N₂O₆

Succinyl acetaminophen

Butanedioic acid, bis[4-(acetylamino)phenyl] ester

Acetanilide, 4'-hydroxy-, succinate

Acetanilide, 4'-hydroxy-, succinate (2:1) (ester)

RN: 2725-63-5 MP (°C): 229–230
MW: 384.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.769E-05	6.800E-03	37	D029	0 0 0 0 0	

4107. C₂₀H₂₀N₆O₆S₂

2,5-Di-(N4-acetylulfanilylamino)pyrimidine

RN: MP (°C):
MW: 504.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.910E-06	5.000E-03	37	R076	1 2 0 0 1	

4108. C₂₀H₂₁ClO₄

Fenofibrate

Proctofene

Sedufen

RN: 49562-28-9 **MP (°C):**
MW: 360.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.217E-06	8.000E-04	25	J415	0 0 0 0 0	

4109. C₂₀H₂₁NO₄

Papaverine

Pantoyl taurine

RN: 58-74-2 **MP (°C):** 147
MW: 339.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-04	3.733E-02	37.5	L034	2 2 0 1 2	pH 7.4

4110. C₂₀H₂₁NO₅

Aspirin phenylalanine ethyl ester

L-Phenylalanine, *N*-[2-(acetoxy)benzoyl]-, ethyl ester

RN: 76748-72-6 **MP (°C):**
MW: 355.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-04	1.670E-01	25	B182	2 2 1 1 1	

4111. C₂₀H₂₁NO₅

Repiprinast

Isoamyl 5,6-dihydro-7,8-dimethyl-4,5-dioxo-4H-pyranos(3,2-c)quinoline-2-carboxylate

RN: 73080-51-0 **MP (°C):**
MW: 355.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.377E-06	1.200E-03	ns	S470	0 0 0 0 0	

4112. C₂₀H₂₂ClN

Pyrrobutamine

Pyrrolidine, 1-[4-(4-chlorophenyl)-3-phenyl-2-butenyl]-

RN: 91-82-7 MP (°C):

MW: 311.86 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.700E-04	2.713E-01	37.5	L034	2 2 0 1 2	pH 7.4

4113. C₂₀H₂₂FN₃O₇

3-Quinolinecarboxylic acid

7-[4-[(acetoxy)methoxy]carbonyl]-1-piperazinyl]-1-ethyl-6-fluoro-1,4-dihydro-4-oxo-

RN: 99106-30-6 MP (°C):

MW: 435.41 BP (°C): 636.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.445E-04	1.500E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
1.378E-04	6.000E-02	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer (0.1 M)
6.890E-05	3.000E-02	25	A414	1 0 1 1 1	pH 5 phosphate buffer (0.1 M)

4114. C₂₀H₂₂N₂O₂

Quininone

Chininon

Cinchonan-9-one, 6'-methoxy-, (8α)-

RN: 84-31-1 MP (°C): 212

MW: 322.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.305E-06	3.000E-03	20	F300	1 0 0 0 0	

4115. C₂₀H₂₂N₈O₅

Methotrexate

(+)-4-Amino-10-methylfolic acid

Metatrexan

Methoblastin

Maxtrex

Ledertrexate

RN: 59-05-2 MP (°C): 195

MW: 454.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.290E+00	1.950E+03	c	B443	0 0 0 0 0	
2.200E-05	1.000E-02	ns	K444	0 0 0 0 0	

4116. C₂₀H₂₃N

Maprotiline

Maprotyline

RN: 10262-69-8 **MP (°C):**
MW: 277.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-06	8.334E-04	22.5	B440	0 0 0 0 0	

4117. C₂₀H₂₃NO₂

Dexoxadrol

(+) -2-(2,2-Diphenyl-1,3-dioxolan-4-yl)piperidine

Relane

CL 911C

RN: 4741-41-7 **MP (°C):**
MW: 309.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.262E-04	7.000E-02	rt	K017	0 2 2 2 2	intrinsic

4118. C₂₀H₂₃N₇O₇

N5-Formyltetrahydropteroylglutamic acid

RN: 58-05-9 **MP (°C):**
MW: 473.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.85E+00	>1.35E+03	25	B443	0 0 0 0 0	

4119. C₂₀H₂₄ClN₃S

Prochlorperazine

Compazine

Ultrazine

Cotranzine

Compa-Z

RN: 58-38-8 **MP (°C):** 228
MW: 373.95 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.496E-02	24	G022	2 0 1 1 1	

4120. C₂₀H₂₄N₂

Dimethindene

Dimetindene

Pyridine, 2-[1-[2-[2-(dimethylamino)ethyl]inden-3-yl]ethyl]-

RN: 5636-83-9 **MP (°C):****MW:** 292.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.160E-04	2.386E-01	37	L094	2 0 0 1 2	pH>10.03, intrinsic

4121. C₂₀H₂₄N₂O₂

Quinine

Chinin

Quinine alkaloid

RN: 130-95-0 **MP (°C):** 177**MW:** 324.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.541E-03	5.000E-01	15	F300	1 0 0 0 0	
9.555E-05	3.100E-02	22	M459	0 0 0 0 0	
1.760E-03	5.711E-01	25	D004	0 0 0 0 0	
9.247E-04	3.000E-01	25	P015	0 0 0 0 0	
4.007E-03	1.300E+00	100	F300	1 0 0 0 1	
<3.08E-04	<1.00E-01	rt	B435	0 0 0 0 0	
1.756E-03	5.697E-01	rt	D021	0 0 1 1 1	

4122. C₂₀H₂₄N₂O₂

Quinidine

Chinidin

Cinchonan-9-ol, 6'-methoxy-, (9S)-

RN: 56-54-2 **MP (°C):** 174**MW:** 324.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-04	2.336E-01	15	K059	2 2 2 0 1	
1.110E-04	3.600E-02	22	M459	0 0 0 0 0	
4.315E-04	1.400E-01	25	F300	1 0 0 0 1	
1.540E-03	4.998E-01	c	D004	0 0 0 0 0	
3.848E-03	1.248E+00	h	D004	0 0 0 0 0	
1.549E-03	5.025E-01	ns	R427	0 0 0 0 0	

4123. C₂₀H₂₄N₂O₂.3H₂O

Quinine (trihydrate)

Quinine, compd. with valeric acid (1:1), hydrate

Cinchonan-9-ol, 6'-methoxy-, trihydrate, (8α,9R)-

RN: 6151-51-5 MP (°C): 57

MW: 378.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.693E-03	6.406E-01	c	D004	0 0 0 0 0	
3.299E-03	1.248E+00	h	D004	0 0 0 0 0	

4124. C₂₀H₂₄N₂O₄

Pheniramine maleate

1-Phenyl-1-(2-pyridyl)-3-dimethylaminopropane maleate

Prophenpyridamine maleate

RN: 132-20-7 MP (°C):

MW: 356.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-02	1.105E+01	37.5	L034	2 2 0 1 2	pH 7.4

4125. C₂₀H₂₄N₂O₅

Naproxen, N-methyl-N-carbamoyl methyl-glycolamide ester

RN: MP (°C): 179.5

MW: 372.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.584E-04	5.900E-02	21	B331	1 2 2 1 1	pH 7.4

4126. C₂₀H₂₄O₃

Methylsecodione

RN: 80702-24-5 MP (°C):

MW: 312.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.919E-03	5.996E-01	25	P324	0 0 0 0 0	

4127. C₂₀H₂₄O₄3,11-Dioxo-4,17(20)-*cis*-pregnadien-21-oic acid methyl ester

U-2726

RN: MP (°C):
MW: 328.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.309E-05	4.300E-03	ns	K029	0 0 2 1 1	

4128. C₂₀H₂₄O₆

Dibenzo-18-crown-6

DBC

RN: 14187-32-7 MP (°C):
MW: 360.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.025E-05	7.300E-03	25	M127	1 2 1 1 1	
9.000E-05	3.244E-02	26	P029	0 0 0 0 0	

4129. C₂₀H₂₅ClN₂O₂

Quinine hydrochloride

Inchonan-9-ol, 6'-methoxy-, monohydrochloride, (8α,9R)-

RN: 130-89-2 MP (°C):
MW: 360.89 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.523E-03	5.497E-01	25	A412	1 0 2 2 1	int

4130. C₂₀H₂₅ClO₂1-Chloro-1,1-dimethyl-2,2-bis(*p*-ethoxylphenyl)ethane

RN: 56265-24-8 MP (°C):
MW: 332.87 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.708E-07	1.900E-04	rt	C122	0 0 0 0 0	

4131. C₂₀H₂₅NO₂

Adiphenine

2-Diethylaminoethyl diphenylacetate

Tranzetil

Patrovine

SKF 962A

RN: 64-95-9

MP (°C): 113.5

MW: 311.43

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-02	3.114E+00	30	L068	1 0 0 1 0	EFG

4132. C₂₀H₂₅NO₄2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-(diethylamino)-2-oxoethyl ester, (S)Naproxen, *N,N*-diethyl glycolamide ester2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-(diethylamino)-2-oxoethyl esterNaproxen *N,N*-diethyl glycolamide ester

RN: 106231-74-7 MP (°C): 89

MW: 343.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.494E-05	1.200E-02	21	B331	1 2 2 1 1	pH 7.4
3.494E-05	1.200E-02	21	B331	0 0 0 0 0	

4133. C₂₀H₂₅NO₄3,11-Dioxo-4,17(20)-*cis*-pregnadien-20-oic acid methyl ester 3-oxime

RN: MP (°C):

MW: 343.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.543E-05	5.300E-03	ns	K029	0 0 2 1 1	

4134. C₂₀H₂₅NO₅Naproxen, *N*-methyl-*N*-hydroxyethyl glycolamide ester

RN: MP (°C): 110

MW: 359.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.895E-04	1.400E-01	21	B331	1 2 2 1 1	pH 7.4

4135. C₂₀H₂₅NO₆2-Naphthaleneacetic acid, 6-methoxy- α -methyl-, 2-[bis(2-hydroxyethyl)amino]-2-oxoethyl ester

Naproxen N,N-diethanol glycolamide ester

Naproxen, N,N-dihydroxyethyl glycolamide ester

RN: 114665-20-2 **MP (°C):** 113**MW:** 375.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.092E-03	4.100E-01	21	B331	1 2 2 1 1	pH 7.4
1.092E-03	4.100E-01	21	B331	0 0 0 0 0	

4136. C₂₀H₂₆N₂

1-(Diphenylmethyl)-4-propylpiperazine

RN: **MP (°C):****MW:** 294.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.448E-04	1.899E-01	25	M438	0 0 0 0 0	

4137. C₂₀H₂₆N₂O₂

Ajmaline

Rauwolfine

Ajmalan-17,21-diol, (17R,21 α)-

Merabitol

Raugalline

RN: 4360-12-7 **MP (°C):** 159**MW:** 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-03	3.591E-01	0	M106	2 1 1 1 0	EFG
1.300E-03	4.244E-01	15	M106	2 1 1 1 0	EFG
1.500E-03	4.897E-01	30	M106	2 1 1 1 0	EFG

4138. C₂₀H₂₆N₂O₂

Hydroquinine

Cinchonan-9-ol, 10,11-dihydro-6'-methoxy-, (8 α ,9R)-

10,11-Dihydroquinine

RN: 522-66-7 **MP (°C):** 173.5**MW:** 326.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.063E-04	9.999E-02	20	K059	2 2 2 0 1	
>1.53E-03	>5.00E-01	ns	B404	0 2 1 1 0	

4139. C₂₀H₂₆O₂

Norethindrone

Norethisterone

RN: 68-22-4

MP (°C): 203

MW: 298.43

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.334E-05	3.981E-03	10	L078	1 0 1 2 0	EFG
1.679E-05	5.012E-03	20	L078	1 0 1 2 0	EFG
2.360E-05	7.043E-03	25	H099	1 0 2 2 2	
1.884E-05	5.623E-03	25	L078	1 0 1 2 2	
8.377E-03	2.500E+00	25	P312	0 0 0 0 0	
2.114E-05	6.310E-03	30	L078	1 0 1 2 0	EFG
3.610E-05	1.077E-02	37	C004	0 0 0 0 0	EFG
2.986E-05	8.912E-03	40	L078	1 0 1 2 0	EFG
4.218E-05	1.259E-02	50	L078	1 0 1 2 0	EFG
3.351E-05	1.000E-02	ns	K444	0 0 0 0 0	

4140. C₂₀H₂₆O₂1,1-Dimethyl-2,2-bis(*p*-ethoxylphenyl)ethane

RN: 56265-21-5 MP (°C):

MW: 298.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.441E-07	4.300E-05	rt	C122	0 0 0 0 0	

4141. C₂₀H₂₆O₄

Dicyclohexyl phthalate

1,2-Benzenedicarboxylic acid, dicyclohexyl ester

RN: 84-61-7 MP (°C): 66

MW: 330.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.211E-05	4.000E-03	24	H116	2 1 0 0 2	

4142. C₂₀H₂₇NO₅S₂2-(Acetyloxy)-4-[2-({5-[(3*R*)-1,2-dithiolan-3-yl]-pentanoyl}-amino)ethyl]phenyl acetate

RN: MP (°C):

MW: 425.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.151E-04	4.900E-02	ns	S453	0 0 0 0 0	

4143. C₂₀H₂₇NO₁₁

Amygdalin

(R)-Amygdalin

(R)-Laenitrile

(R)-Amygdaloside

RN: 29883-15-6 MP (°C): 223

MW: 457.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.705E-01	7.800E+01	10	F300	1 0 0 0 1	
1.698E-01	7.768E+01	ns	R427	0 0 0 0 0	

4144. C₂₀H₂₇NO₁₁.3H₂O

Amygdalin (trihydrate)

D-(–)-Amygdalin

(R)-Amygdalin

RN: 29883-15-6 MP (°C): 214–216

MW: 511.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.504E-01	7.692E+01	c	D004	0 0 0 0 0	
		h	D004	0 0 0 0 0	

4145. C₂₀H₂₇O₄P

Octyldiphenyl phosphate

Disflamoll DPO

RN: 115-88-8 MP (°C):

MW: 362.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.863E-07	1.400E-04	24	H116	2 1 0 0 2	

4146. C₂₀H₂₈O

Vitamin A aldehyde

Retinal

All-*trans*-retinalAll-*trans* vitamin A aldehyde

Retinene

RN: 116-31-4 MP (°C): 63

MW: 284.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.46E-04	<7.00E-02	25	P312	0 0 0 0 0	

4147. C₂₀H₂₈O₂

19-Norprogesterone

19-Norpregn-4-ene-3,20-dione

RN: 472-54-8 MP (°C):

MW: 300.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-04	3.610E-02	37	L010	2 0 2 1 1	

4148. C₂₀H₂₈O₂

Retinoic acid

All-*trans* retinoic acid

3,7-Dimethyl-9-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonenatetraenoic acid

β-All-*trans*-retinoic acid

RN: 302-79-4 MP (°C): 180-181

MW: 300.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.33E-04	<7.00E-02	25	P312	0 0 0 0 0	

4149. C₂₀H₂₈O₃

5,6-Dehydroisoandrosterone formate

Androst-5-en-17-one, 3α-hydroxy-, formate

RN: 4589-84-8 MP (°C):

MW: 316.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.424E-05	1.400E-02	ns	B057	0 2 1 1 2	

4150. C₂₀H₂₈O₃

Testosterone formate

Androst-4-en-17β-ol-3-one formate

Testosterone 17-formate

RN: 3129-42-8 MP (°C):

MW: 316.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.389E-05	4.395E-03	25	J004	1 0 1 1 2	
1.390E-05	4.400E-03	ns	B057	0 2 1 1 1	

4151. C₂₀H₂₉N₃O₂

Dibucaine

Cinchocaine

RN: 85-79-0**MP (°C):** 64**MW:** 343.47**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.980E-04	6.801E-02	ns	B018	0 0 0 0 2	
1.980E-04	6.801E-02	ns	M066	0 0 0 0 2	

4152. C₂₀H₃₀N₄O₆

2'-Nonyl-6-methoxypurine arabinoside

4-Quinolinecarboxamide, 2-butoxy-*N*-[2-(diethylamino)ethyl]-**RN:** 145913-42-4 **MP (°C):** 88-90**MW:** 422.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.030E-04	4.352E-02	37	C348	0 0 0 0 0	pH 7.00

4153. C₂₀H₃₀O

D 263

4,6-Diisopropyl-1,1-dimethyl-7-propionylindan

RN: 290294-31-4 **MP (°C):** 117**MW:** 286.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.491E-06	1.000E-03	ns	M061	0 0 0 0 0	

4154. C₂₀H₃₀O

Vitamin A

Retinol

Afinaxin

α-Sterol

RN: 68-26-8 **MP (°C):** 62**MW:** 286.46 **BP (°C):** 137-138

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<3.49E-05	<1.00E-02	25	P312	0 0 0 0 0	

4155. C₂₀H₃₀O₂

Abietic acid

13-Isopropylpodocarpa-7,13-dien-15-oic acid

Sylvic acid

RN: 514-10-3 MP (°C): 172

MW: 302.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	4.839E-02	20	B009	2 2 1 2 0	

4156. C₂₀H₃₀O₂

17-Methyltestosterone

17- α -Methyltestosterone

Methyltestosterone

Methyl-testosterone

RN: 58-18-4 MP (°C): 161

MW: 302.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.230E-04	3.720E-02	20	F012	1 0 1 1 1	
1.120E-04	3.388E-02	25	H099	1 0 2 2 2	
1.058E-04	3.200E-02	25	K003	2 1 1 1 1	
4.400E-02	1.331E+01	25	M379	1 0 1 1 0	EFG, <i>sic</i>
<5.62E-04	<1.70E-01	25	P312	0 0 0 0 0	
2.313E-03	6.995E-01	25	P324	0 0 0 0 0	
1.018E-04	3.080E-02	30	T005	2 0 2 2 2	
1.200E-04	3.630E-02	37	E014	2 2 2 1 2	pH 7.3
7.472E-05	2.260E-02	ns	B057	0 2 1 1 2	
9.918E-05	3.000E-02	rt	N302	0 2 1 2 1	

4157. C₂₀H₃₀O₃

Androstanolone formate

5 α -Androstan-3-one, 17-hydroxy-, formate

RN: 4589-90-6 MP (°C):

MW: 318.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.679E-06	1.490E-03	ns	B057	0 2 1 1 2	

4158. C₂₀H₃₀O₆

Butyl glycol phthalate
 bis(2-Butoxyethyl) phthalate
 Dibutoxyethyl phthalate
 bis(2-N-Butoxyethyl) phthalate

RN: 117-83-9 **MP (°C):** 230
MW: 366.46 **BP (°C):** 210

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.458E-05	2.000E-02	15	H069	1 0 1 1 0	
<8.18E-04	<3.00E-01	20	F070	1 0 0 0 1	

4159. C₂₀H₃₁NO

Trihexyphenidyl
 1-Phenyl-1-cyclohexyl-3-piperidyl-1-propanol hydrochloride

Artane
 Benzhexol chloride
 Trihexyphenidyl-D,L hydrochloride
 Tremin

RN: 52-49-3 **MP (°C):**
MW: 301.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.226E-06	6.709E-04	22.5	B440	0 0 0 0 0	

4160. C₂₀H₃₁NO₃

Acetaminophen laurate
 Acetaminophen dodecanoate

RN: 54942-38-0 **MP (°C):** 111
MW: 333.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.799E-05	6.000E-03	25	B010	1 1 1 1 0	

4161. C₂₀H₃₂O₃

Tridecyl *p*-hydroxybenzoate
p-Hydroxybenzoic acid tridecyl ester

RN: 69679-32-9 **MP (°C):**
MW: 320.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.135E-03	3.639E-01	25	D081	1 2 2 1 2	

4162. C₂₀H₃₂O₅

Dinoprostone
Prostaglandin E2

RN: 363-24-6 **MP (°C):** 66–68
MW: 352.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.123E-03	1.101E+00	8.53	F068	0 0 2 2 0	
4.022E-03	1.418E+00	19.24	F068	0 0 2 2 0	
4.173E-03	1.471E+00	25.35	F068	0 0 2 2 0	
4.575E-03	1.613E+00	29.9	F068	0 0 2 2 0	

4163. C₂₀H₃₃NO

Fenpropimorph

4-(3-(4-(1,1-Dimethylethyl)phenyl)-2-methylpropyl)-2,6-dimethylmorpholine

Corbe

Mistral

RN: 67306-03-0 **MP (°C):**
MW: 303.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.417E-05	4.300E-03	ns	V414	0 0 0 0 0	

4164. C₂₀H₃₃NO₃

4-Heptoxybenzoic acid-2-(diethyl-amino)ethyl ester

RN: 38973-75-0 **MP (°C):**
MW: 335.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	1.677E-02	ns	M066	0 0 0 0 1	

4165. C₂₀H₃₃N₃O₄

Celiprolol

RN: 56980-93-9 **MP (°C):**
MW: 379.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.034E-05	2.290E-02	22.5	B440	0 0 0 0 0	
6.008E-09	2.280E-06	200	M418	0 0 0 0 0	

4166. C₂₀H₃₄

5-Phenyltetradecane

RN:**MW:** 274.49**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.372E-06	25	S377	0 0 0 0 0	

4167. C₂₀H₃₄

2-Phenyltetradecane

RN:**MW:** 274.49**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4168. C₂₀H₃₄

4-Phenyltetradecane

RN:**MW:** 274.49**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4169. C₂₀H₃₄

3-Phenyltetradecane

RN:**MW:** 274.49**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.372E-06	25	S377	0 0 0 0 0	

4170. C₂₀H₃₄

6-Phenyltetradecane

RN:**MW:** 274.49**MP (°C):****BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-09	1.098E-06	25	S377	0 0 0 0 0	

4171. C₂₀H₃₄N₂O₂

4-Heptylaminobenzoic acid-2-(diethyl-amino)ethyl ester

RN: **MP (°C):**
MW: 334.51 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-04	7.025E-02	ns	M066	0 0 0 0 1	

4172. C₂₀H₃₄O₄

4-Octylphenol triethoxylate

RN: 51437-91-3 **MP (°C):**
MW: 338.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.436E-05	1.840E-02	20.5	A335	0 0 0 0 0	
5.440E-05	1.841E-02	20.5	A335	0 0 0 0 0	

4173. C₂₀H₃₄O₈

Acetyl tributyl citrate

1,2,3-Propanetricarboxylic acid

Tributyl acetylcitrate

RN: 77-90-7 **MP (°C):**
MW: 402.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.224E-06	1.700E-03	25	F067	1 0 2 2 1	

4174. C₂₀H₃₆O₄

Diocyl maleate

2-Butenedioic acid (Z)-

Diocyl ester

RN: 2915-53-9 **MP (°C):**
MW: 340.51 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.762E-06	6.000E-04	25	F067	1 0 2 2 2	

4175. C₂₀H₃₆O₆

Dicyclohexyl-18-crown-6

Dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin, icosahydro-

Dicyclohexano-18-crown-6

cis-Dicyclohexano-18-crown-6**RN:** 16069-36-6 **MP (°C):****MW:** 372.51 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.600E-02	1.341E+01	26	P029	0 0 0 0 0	
2.200E-02	8.195E+00	53	P029	0 0 0 0 0	
1.000E-02	3.725E+00	82	P029	0 0 0 0 0	

4176. C₂₀H₄₀

1-Eicosene

n-Eicosene**RN:** 3452-07-1 **MP (°C):****MW:** 280.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.907E-12	5.350E-10	23	C332	0 0 0 0 0	

4177. C₂₁H₁₁ClF₆N₂O₃

Flufenoxuron

RN: 101463-69-8 **MP (°C):****MW:** 488.78 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.775E-09	3.800E-06	20	M402	0 0 0 0 0	

4178. C₂₁H₁₃N

1:2,6:7-Dibenzacridine

RN: 226-92-6 **MP (°C):****MW:** 279.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.397E-05	22	B175	1 0 1 1 0	

4179. C₂₁H₁₃N

1:2,8:9-Dibenzacridine

RN: 224-53-3 **MP (°C):****MW:** 279.34 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-08	1.955E-05	22	B175	1 0 1 1 0	

4180. C₂₁H₁₃N

3:4,6:7-Dibenzacridine

RN: 226-97-1

MP (°C):

MW: 279.34

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-07	6.984E-05	22	B175	1 0 1 1 1	

4181. C₂₁H₁₄

5-Methyl-3,4-benzpyrene

RN: 31647-36-6

MP (°C): 216

MW: 266.35

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-09	8.000E-07	27	D003	1 0 0 1 0	

4182. C₂₁H₁₅CIN₂O₄S1-(*p*-Chlorobenzenesulfonyl)-5,5-diphenyl-hydantoin

RN: 24759-38-4

MP (°C):

MW: 426.88

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.965E-07	3.400E-04	37	F183	1 0 1 1 2	intrinsic

4183. C₂₁H₁₅N₃O₆S1-(*p*-Nitrobenzenesulfonyl)-5,5-diphenyl-hydantoin

RN: 21413-53-6

MP (°C):

MW: 437.43

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.486E-06	6.500E-04	37	F183	1 0 1 1 2	intrinsic

4184. C₂₁H₁₆

3-Methylcholanthrene

1,2-Dihydro-3-methyl-benz[j]aceanthrylene

20-Methylcholanthrene

RN: 56-49-5

MP (°C): 179

MW: 268.36

BP (°C): 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.204E-08	3.230E-06	24	H106	1 0 2 2 2	
1.081E-08	2.900E-06	25	M064	1 1 2 2 1	
1.204E-08	3.230E-06	25	M156	1 2 1 1 2	
1.100E-08	2.952E-06	25	M342	1 0 1 1 1	
5.589E-09	1.500E-06	27	D003	1 0 0 1 1	
1.081E-08	2.900E-06	ns	M344	0 0 0 0 1	

4185. C₂₁H₁₆N₂O₂

C.I. Disperse blue 24

9,10-Anthracenedione, 1-amino-4-hydroxy-2-phenoxy-

Serilene red 2BL

Sumikaron red E-FBL

Solvent red 146

RN: 17418-58-5 MP (°C): 151

MW: 328.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-08	1.642E-05	25	B333	0 0 0 0 0	

4186. C₂₁H₁₆N₂O₄S

1-Benzenesulfonyl-5,5-diphenyl-hydantoin

RN: 21413-28-5 MP (°C):

MW: 392.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.587E-06	1.800E-03	37	F183	1 0 1 1 2	intrinsic

4187. C₂₁H₁₆N₂O₅S1-(*p*-Hydroxylbenzenesulfonyl)-5,5-diphenyl-hydantoin

RN: 24759-35-1 MP (°C):

MW: 408.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.080E-06	3.300E-03	37	F183	1 0 1 1 2	intrinsic

4188. C₂₁H₁₇N₃O₂S₂2-Sulfanilamido-4-*p*-diphenylthiazole

RN: MP (°C):

MW: 407.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.454E-06	1.000E-03	37	R045	1 2 1 1 0	

4189. C₂₁H₁₇N₃O₄S1-(*p*-Aminobenzenesulfonyl)-5,5-diphenyl-hydantoin

RN: 24759-34-0 MP (°C):

MW: 407.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.436E-06	1.400E-03	37	F183	1 0 1 1 2	intrinsic

4190. C₂₁H₁₉NO₄

Cinmetacin

1-Cinnamoyl-2-methyl-5-methoxyindolyl-3-acetic acid

Indolacin

RN: 20168-99-4 **MP (°C):** 170**MW:** 349.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.86E-06	<1.00E-03	25	K027	2 0 2 2 0	

4191. C₂₁H₂₀Cl₂O₃

Permethrin

3-(2,2-Dichloroethyl)-2,2-dimethylcyclopropanecarboxylic acid (3-phenoxyphenyl)methyl Ester

Ambush

Pounce

Ectiban

RN: 52645-53-1 **MP (°C):** 36.5**MW:** 391.30 **BP (°C):** 200

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.111E-07	2.000E-04	ns	M161	0 0 0 0 0	
~5.11E-07	~2.00E-04	ns	Y418	0 0 0 0 0	

4192. C₂₁H₂₀O₉

Puerarin

8-β-D-Glucopyransyl-7-hydroxy-3-(4-hydroxyphenyl)-4H-1benzopyran-4-one

RN: 3681-99-0 **MP (°C):****MW:** 416.39 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-01	3.373E+02	15.0	W418	0 0 0 0 0	
9.500E-01	3.956E+02	20.0	W418	0 0 0 0 0	
1.100E+00	4.580E+02	25.0	W418	0 0 0 0 0	
1.260E+00	5.246E+02	30.0	W418	0 0 0 0 0	
1.420E+00	5.913E+02	35.0	W418	0 0 0 0 0	
1.710E+00	7.120E+02	40.0	W418	0 0 0 0 0	
2.020E+00	8.411E+02	45.0	W418	0 0 0 0 0	
2.430E+00	1.012E+03	50.0	W418	0 0 0 0 0	
2.840E+00	1.183E+03	55.0	W418	0 0 0 0 0	

4193. C₂₁H₂₁ClN₂O₈

Demeclocycline

Declomycin

Methylchlorotetracycline

Demethylchlortetracycline

RN: 127-33-3 **MP (°C):****MW:** 464.86 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.259E-03	1.515E+00	21	M044	2 0 2 2 2	
3.012E-03	1.400E+00	25	B191	1 0 0 0 1	neutral pH

4194. C₂₁H₂₁N

Cyproheptadine

RN: 129-03-3 **MP (°C):****MW:** 287.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	3.176E-04	22.5	B440	0 0 0 0 0	

4195. C₂₁H₂₁NO₆

Rhoeadine

[1,3]Dioxolo[4,5-h]-1,3-dioxolo[7,8][2]benzopyrano[3,4-a][3]benzazepine, 5β,6,7,8,13β,15-hexahydro-15-methoxy-6-methyl-, (5b*R*,13b*R*,15*S*)

8-Methoxy-16-methyl-2,3:10,11-bis[methylenebis(oxy)]-, (8β)-

RN: 2718-25-4 **MP (°C):** 245–247dec**MW:** 383.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.172E-03	8.326E-01	25	D004	0 0 0 0 0	

4196. C₂₁H₂₁NO₆

Hydrastine

Hydrastin

(1*R*,9*S*)-β-Hydrastine**RN:** 118-08-1 **MP (°C):** 132**MW:** 383.40 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-04	3.144E-01	15	K059	2 2 2 0 1	
7.825E-05	3.000E-02	20	F300	1 0 0 0 1	

4197. C₂₁H₂₁N₃O₃S

L-Phe-dapsone

Benzene propanamide, α -amino-*N*-[4-[(4-aminophenyl)sulfonyl]phenyl]-, (*S*)-

RN: 160349-01-9 MP (°C):

MW: 395.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.057E-06	2.000E-03	25	P351	0 0 0 0 0	pH 7.4
3.287E-03	1.300E+00	25	P351	0 0 0 0 0	

4198. C₂₁H₂₁O₄P

Tricresyl phosphate

Tritolyl phosphate

Tri-*p*-cresyl phosphate

RN: 1330-78-5 MP (°C):

MW: 368.37 BP (°C): 265

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.009E-07	7.400E-05	24	H116	2 1 0 0 1	
2.715E-07	1.000E-04	25	F067	1 0 2 2 1	
2.172E-04	7.999E-02	ns	F014	0 0 0 0 0	

4199. C₂₁H₂₂N₂O₂

Strychnine

Strychnidin-10-one

Gopher Getter

L-Strychnine

Gopher Bait

RN: 57-24-9 MP (°C): 275

MW: 334.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	9.029E-02	15	K059	2 2 2 0 1	
4.186E-04	1.400E-01	20.0	N002	2 1 2 2 1	
5.980E-04	2.000E-01	30.0	N002	2 1 2 2 1	
1.017E-03	3.400E-01	40.0	N002	2 1 2 2 1	
1.196E-03	4.000E-01	50.0	N002	2 1 2 2 1	
1.346E-03	4.500E-01	60.0	N002	2 1 2 2 1	
1.794E-03	6.000E-01	75.0	N002	2 1 2 2 1	
4.672E-04	1.562E-01	c	D004	0 0 0 0 0	
9.643E-04	3.225E-01	h	D004	0 0 0 0 0	
4.276E-04	1.430E-01	rt	M161	0 0 0 0 2	

4200. C₂₁H₂₂N₂O₅

Benzeneacetic acid, 4-benzoyl- α -methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester

N-Methyl-*N*-carbamoyl methyl glycolamide salicylate

RN: 114665-16-6 **MP (°C):** 83

MW: 382.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.792E-03	1.450E+00	21	B331	0 0 0 0 0	

4201. C₂₁H₂₂N₂O₅

Ketoprofen, *N*-methyl-*N*-carbamoylmethyl glycolamide ester

Benzeneacetic acid, 3-benzoyl- α -methyl-, 2-[(2-amino-2-oxoethyl)methylamino]-2-oxoethyl ester

RN: 116482-84-9 **MP (°C):** 83.5

MW: 382.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.792E-03	1.450E+00	21	B331	1 2 2 1 1	pH 7.4

4202. C₂₁H₂₃CIFNO₂

Haloperidol

Haldol

4-[4-(*p*-Chlorophenyl)-4-hydroxypiperidino]-4'-fluorobutyrophenone

Serenace

RN: 52-86-8 **MP (°C):** 148

MW: 375.87 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.623E-04	6.100E-02	22	J420	0 0 0 0 0	pH6.5
5.474E-06	2.058E-03	22.5	B440	0 0 0 0 0	
7.981E-06	3.000E-03	30	P044	0 0 0 0 0	
2.660E-05	1.000E-02	ns	K444	0 0 0 0 0	
<2.66E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4203. C₂₁H₂₃N₃OS

Pericyazine

2-Cyano-10-[3'-(4"-hydroxypiperidino)propyl]phenothiazine

Periciazine

RN: 2622-26-6 **MP (°C):** 116

MW: 365.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E-04	3.801E-02	37	F011	1 0 1 1 2	pH 7.4

4204. C₂₁H₂₄FN₃O₇

3-Quinolinecarboxylic acid

7-[4-[[1-(Acetoxy)ethoxy]carbonyl]-1-piperazinyl]-1-ethyl-6-fluoro-1,4-dihydro-4-oxo-

RN: 99106-35-1 **MP (°C):** 216
MW: 449.44 **BP (°C):** 636.7

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.122E-04	4.100E-01	25	A414	1 0 1 1 1	pH 8.5 bicarbonate buffer (0.05 M)
1.112E-04	5.000E-02	25	A414	1 0 1 1 1	pH 7.4 phosphate buffer (0.1 M)
1.112E-05	5.000E-03	25	A414	1 0 1 1 1	pH 5 citrate buffer (0.1 M)
1.335E-04	6.000E-02	25	A414	1 0 1 1 1	

4205. C₂₁H₂₄F₃N₃S

Trifluoperazine

Stelazine

RN: 117-89-5 **MP (°C):** 232
MW: 407.50 **BP (°C):** 206

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	1.223E-02	24	G022	2 0 1 1 1	
3.600E-05	1.467E-02	37	F011	1 0 1 1 1	pH 7.4

4206. C₂₁H₂₅NO

4-Cyano-4'-octyloxybiphenyl

8 COB

RN: **MP (°C):**
MW: 307.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-07	8.301E-05	21	D300	2 2 1 1 2	

4207. C₂₁H₂₅N₅O₅

Benzoic acid, 4-(4-morpholinylmethyl)-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c]pyridin-1-yl)methoxy]ethyl ester

1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.

RN: 137605-75-5 **MP (°C):**
MW: 427.46 **BP (°C):** 712.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.801E-03	7.700E-01	21	B419	1 1 2 2 1	int

4208. C₂₁H₂₆ClN₃OS

Perphenazine

4-(3-(2-Chlorophenothiazin-10-YL)propyl)-1-piperazineethanol

Etrafon

Trilafon

RN: 58-39-9**MP (°C):** 97**MW:** 403.98**BP (°C):** 280

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-05	2.828E-02	24	G022	2 0 1 1 1	

4209. C₂₁H₂₆FN₃O₄

Permafloxacin

RN: 143383-65-7 **MP (°C):****MW:** 403.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.853E-02	7.477E+00	25	F415	0 0 0 0 0	Average

4210. C₂₁H₂₆N₂O₃1-(2,3-Dihydro-5-methoxybenzo[b]furan-2-ylmethyl)-4-(*o*-methoxyphenyl)piperazine**RN:** **MP (°C):****MW:** 354.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.642E-05	2.000E-02	37	L079	1 0 1 1 0	intrinsic

4211. C₂₁H₂₆N₂S₂

Thioridazine

10H-Phenothiazine

10-[2-(1-Methyl-2-piperidyl)ethyl]-2-methylthio

Aldazine

Mellaril

Melleril

RN: 50-52-2 **MP (°C):****MW:** 370.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.004E-06	1.113E-03	22.5	B440	0 0 0 0 0	

4212. C₂₁H₂₆O₄

Lifibrol

Benzoic acid, 4-[4-(1,1-dimethylethyl)phenyl]-2-hydroxybutoxy]-

RN: 96609-16-4 **MP (°C):****MW:** 342.44 **BP (°C):** 536.8

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-07	1.301E-04	12.0	B412	1 0 2 2 1	mod 2 crystal
8.600E-07	2.945E-04	12.0	B412	1 0 2 2 1	mod I crystal
7.000E-07	2.397E-04	20.0	B412	1 0 2 2 1	mod 2 crystal
1.110E-06	3.801E-04	20.0	B412	1 0 2 2 1	mod 1 crystal
1.070E-06	3.664E-04	29.0	B412	1 0 2 2 1	mod 2 crystal
1.640E-06	5.616E-04	29.0	B412	1 0 2 2 1	mod 1 crystal
2.090E-06	7.157E-04	38.0	B412	1 0 2 2 1	mod 2 crystal
2.740E-06	9.383E-04	38.0	B412	1 0 2 2 1	mod 1 crystal
3.080E-06	1.055E-03	47.0	B412	1 0 2 2 1	mod 2 crystal
4.890E-06	1.675E-03	47.0	B412	1 0 2 2 1	mod 1 crystal
4.690E-06	1.606E-03	54.0	B412	1 0 2 2 1	mod 2 crystal
5.900E-06	2.020E-03	54.0	B412	1 0 2 2 1	mod 1 crystal

4213. C₂₁H₂₆O₄

17-Hydroxy-6-methyl-16-methylenepregna-4,6-diene-3,20-dione acetate

RN: **MP (°C):****MW:** 342.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.469E-06	2.900E-03	37	H004	0 0 0 0 0	

4214. C₂₁H₂₆O₅

Prednisone

1,4-Pregnadiene-17 α ,21-diol-3,11,20-trione1,4-Pregnadiene-17 α ,21-diol-3,11,20-trione

Delcortin

Metocorten

Panasol

RN: 53-03-2 **MP (°C):** 234**MW:** 358.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.208E-04	1.150E-01	25	K003	2 1 1 1 1	
2.734E-04	9.799E-02	ns	B404	0 2 1 1 0	

4215. C₂₁H₂₇FO₅

Fluprednisolone

6 α -Fluoro-11 β ,17,21-trihydroxypregna-1,4-diene-3,20-dione17,21-trihydroxypregna-1,4-diene-3,20-dione

Alphadrol

RN: 53-34-9**MP (°C):****MW:** 378.44**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.748E-03	1.040E+00	37	H004	0 0 0 0 0	

4216. C₂₁H₂₇FO₅.H₂O

Fluprednisolone (monohydrate)

RN: 53-34-9**MP (°C):****MW:** 396.46**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-03	5.860E-01	37	H004	0 0 0 0 0	

4217. C₂₁H₂₇FO₆

Triamcinolone

9 α -Fluoro-11 β ,16 α ,17 α ,21-tetrahydroxy-1,4-pregnadiene-3,20-dione9 α -Fluoro-16 α -hydroxyprednisolone

Aristocort

RN: 124-94-7**MP (°C):** 269**MW:** 394.44**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.028E-04	7.999E-02	25	F024	1 0 0 0 0	
4.260E-04	1.680E-01	37	C400	2 0 2 2 2	

4218. C₂₁H₂₇NO₃

Propafenone

RN: 54063-53-5**MP (°C):****MW:** 341.45**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.226E-06	7.599E-04	22.5	B440	0 0 0 0 0	

4219. C₂₁H₂₈N₂

1-(Diphenylmethyl)-4-butylpiperazine
RN: **MP (°C):**
MW: 308.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.561E-03	4.816E-01	25	M438	0 0 0 0 0	

4220. C₂₁H₂₈N₄O₇

Pentyloxycarbonyl-mitomycin C
RN: **MP (°C):**
MW: 448.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.900E-04	2.646E-01	25	M316	1 1 1 1 2	

4221. C₂₁H₂₈O₂

Norgestrel
Microlut
Microval
RN: 797-63-7 **MP (°C):** 206
MW: 312.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.200E-05	1.000E-02	ns	K444	0 0 0 0 0	

4222. C₂₁H₂₈O₂

Ethisterone
17 α -Ethynyl testosterone
Ethynyl testosterone
Gestoral
Pregnenolone
Anhydrohydroxyprogesterone
RN: 434-03-7 **MP (°C):** 269
MW: 312.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.920E-06	5.999E-04	20	G072	1 2 2 1 2	
1.600E-06	4.999E-04	20	L077	1 2 2 2 1	
1.280E-06	4.000E-04	25	K003	2 1 1 1 1	
2.200E-06	6.874E-04	27.34	L077	1 2 2 2 1	
3.200E-06	9.999E-04	35	L077	1 2 2 2 1	
3.500E-06	1.094E-03	42.34	L077	1 2 2 2 1	
4.200E-06	1.312E-03	50	L077	1 2 2 2 1	

4223. C₂₁H₂₈O₂1,1,1-Trimethyl-2,2-bis(*p*-ethoxyphenyl)ethane

RN: 27955-87-9 MP (°C):

MW: 312.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.481E-07	1.400E-04	rt	C122	0 0 0 0 0	

4224. C₂₁H₂₈O₅

Prednisolone

11β,17α,21-Trihydroxypregna-1,4-diene-3,20-dione

Ropredlone

Predonin

Hostacortin H

Nisolone

RN: 50-24-8 MP (°C): 240

MW: 360.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.173E-03	2.225E+00	25	G008	1 2 1 1 2	<i>sic</i>
5.963E-04	2.150E-01	25	K003	2 1 1 1 1	
1.379E-03	4.970E-01	25	K021	1 2 2 2 1	
5.770E-04	2.080E-01	25	M457	0 0 0 0 0	
7.000E-04	2.523E-01	30	H016	2 2 2 2 0	EFG
1.268E-03	4.570E-01	30	T002	1 0 2 0 2	anhydrous, form A
1.398E-03	5.040E-01	30	T002	1 0 2 0 2	anhydrous, form B
6.658E-04	2.400E-01	30	T002	1 0 2 0 2	hydrate
6.658E-04	2.400E-01	30	W006	2 2 2 1 2	hydrate, form C
4.694E-04	1.692E-01	37	C400	2 0 2 2 2	
9.738E-04	3.510E-01	37	H004	0 0 0 0 0	
5.500E-04	1.982E-01	ns	F327	0 0 1 2 2	
2.774E-04	1.000E-01	ns	K444	0 0 0 0 0	
1.398E-03	5.040E-01	ns	W006	2 2 2 1 2	anhydrous, form B

4225. C₂₁H₂₈O₅

Aldosterone

18-Oxcorticosterone

Aldocortin

Electrocortin

18-Oxo-11β,21-dihydroxy-4-pregnene-3,20-dione

RN: 52-39-1 MP (°C): 108

MW: 360.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.420E-04	5.118E-02	37	H034	1 0 2 1 2	pH 7.4
1.413E-04	5.092E-02	ns	R427	0 0 0 0 0	

4226. C₂₁H₂₈O₅

Cortisone

17-Hydroxy-11-dehydrocorticosterone

Cortate

RN: 53-06-5**MP (°C):** 222**MW:** 360.45**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.766E-04	2.799E-01	20	D041	1 0 0 0 0	
6.379E-04	2.299E-01	25	K003	2 1 1 1 1	
7.768E-04	2.800E-01	25	M023	1 0 2 1 1	
7.500E-04	2.703E-01	30	L344	2 0 1 1 0	EFG
6.000E-04	2.163E-01	37	E014	2 2 2 1 2	pH 7.3
7.768E-04	2.800E-01	ns	B338	0 0 0 0 1	

4227. C₂₁H₂₉FO₅

Fludrocortisone

9α-Fluoro-17-hydroxycorticosterone

9α-Fluorohydrocortisone

Florinef

RN: 127-31-1**MP (°C):** 260dec**MW:** 380.46**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.918E-04	1.110E-01	25	K021	1 2 2 2 1	
8.516E-04	3.240E-01	25	L009	1 0 0 1 1	
2.411E-04	9.172E-02	37	C400	2 0 2 2 2	

4228. C₂₁H₂₉NO

N,N-Dicyclohexylcinnamamide

N,N-Dicyclohexyl-3-phenyl-2-propenamide

RN: 6631-21-6**MP (°C):****MW:** 311.47**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.680E-06	1.769E-03	ns	H350	0 0 0 0 0	

4229. C₂₁H₂₉N₃O

Disopyramide

α-(2-(Diisopropylamino)ethyl)-α-phenyl-2-pyridineacetamide

RN: 3737-09-5**MP (°C):****MW:** 339.48**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.817E-05	6.170E-03	22.5	B440	0 0 0 0 0	
1.995E-02	6.774E+00	ns	R427	0 0 0 0 0	

4230. C₂₁H₃₀N₄O₁₀

Methylol riboflavin
Methylol-riboflavin

RN: **MP (°C):**
MW: 498.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.387E-02	1.190E+01	20	F300	1 0 0 0 2	compound not stable

4231. C₂₁H₃₀N₆O₄S

Benzenesulfonamide, N-[2-(dimethylamino)ethyl]-4-(2,3,4,5,6,7-hexahydro-2,6-dioxo-1,3-dipropyl-1H-purin-8-yl)-

RN: 89073-58-5 **MP (°C):** 270dec
MW: 462.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.302E-02	1.990E+01	ns	H316	0 0 0 0 0	0.1N HCL
1.081E-04	5.000E-02	ns	H316	0 0 0 0 0	pH 7.4

4232. C₂₁H₃₀O₂

Tetrahydrocannabinol

THC

Dronabinol

89-Tetrahydrocannabinol

RN: 1972-08-3 **MP (°C):**
MW: 314.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.904E-06	2.800E-03	23	G018	1 0 0 1 0	

4233. C₂₁H₃₀O₂

Progesterone

84-Pregnene-3,20-dione

Corlutin

Corlutina

Lutein

Pregn-4-ene-3,20-dione

RN: 57-83-0 **MP (°C):** 121
MW: 314.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-05	5.346E-03	10	B012	2 0 1 1 0	
2.200E-05	6.918E-03	20	B012	2 0 1 1 0	
3.210E-05	1.009E-02	20	L077	1 2 2 2 2	
2.600E-05	8.176E-03	21.70	M108	1 2 1 1 2	form A (continued)

4233. C₂₁H₃₀O₂ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.837E-05	1.521E-02	23	B014	0 0 1 2 2	
3.720E-05	1.170E-02	24.00	M108	1 2 1 1 2	form B
2.800E-05	8.805E-03	25	B012	2 0 1 1 0	
2.512E-05	7.899E-03	25	B041	1 0 2 2 0	EFG
3.802E-05	1.196E-02	25	F312	1 1 2 2 2	units assumed
2.862E-05	9.000E-03	25	K003	2 1 1 1 1	
6.359E-04	2.000E-01	25	P324	0 0 0 0 0	
2.810E-05	8.837E-03	25.30	M108	1 2 1 1 2	form A
3.690E-05	1.160E-02	27.34	L077	1 2 2 2 2	
3.600E-05	1.132E-02	30	B012	2 0 1 1 0	
3.498E-05	1.100E-02	30	M007	2 2 1 2 2	average of 8
3.800E-05	1.195E-02	30.20	M108	1 2 1 1 2	form A
4.520E-05	1.421E-02	30.50	M108	1 2 1 1 2	form B
4.230E-05	1.330E-02	35	L077	1 2 2 2 2	
5.390E-05	1.695E-02	35.50	M108	1 2 1 1 2	form B
4.690E-05	1.475E-02	36.40	M108	1 2 1 1 2	form A
3.816E-05	1.200E-02	37	A086	1 0 1 1 2	
3.528E-05	1.109E-02	37	C400	2 0 2 2 2	
4.800E-05	1.509E-02	37	H034	1 0 2 1 2	pH 7.4
4.260E-05	1.340E-02	37	H035	1 1 1 1 2	pH 7.4
4.007E-05	1.260E-02	37	L010	2 0 2 1 1	
4.260E-05	1.340E-02	37.50	B041	1 0 2 2 2	
3.981E-05	1.252E-02	37.50	B041	1 0 2 2 0	EFG
3.800E-05	1.195E-02	40	B012	2 0 1 1 0	
6.750E-05	2.123E-02	40.70	M108	1 2 1 1 2	form B
6.370E-05	2.003E-02	41.30	M108	1 2 1 1 2	form A
4.580E-05	1.440E-02	42.34	L077	1 2 2 2 2	
6.500E-05	2.044E-02	46.10	M108	1 2 1 1 2	form A
4.900E-05	1.541E-02	50	B012	2 0 1 1 0	
4.930E-05	1.550E-02	50	L077	1 2 2 2 2	
		amb	L434	0 0 0 0 0	
1.908E-05	6.000E-03	ns	B404	0 2 1 1 0	

4234. C₂₁H₃₀O₃

Deoxycorticosterone

21-Hydroxyprogesterone

4-Pregnen-21-ol-3,20-dione

11-Deoxycorticosterone

21-Hydroxypregn-4-ene-3,20-dione

RN: 64-85-7 MP (°C): 141.5

MW: 330.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.387E-04	1.450E-01	25	K003	2 1 1 1 1	
4.588E-04	1.516E-01	37	C400	2 0 2 2 2	
1.800E-04	5.948E-02	37	E014	2 2 2 1 2	pH 7.3
1.070E-04	3.536E-02	37	H034	1 0 2 1 2	pH 7.4

4235. C₂₁H₃₀O₃

11α-Hydroxyprogesterone

11α-Hydroxy-4-pregnene-3,20-dione

RN: 80-75-1 MP (°C):

MW: 330.47 BP (°C): 165–166

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.522E-04	1.164E-01	37	C400	2 0 2 2 2	

4236. C₂₁H₃₀O₃

11β-Hydroxyprogesterone

11β-Hydroxypregn-4-ene-3,20-dione

RN: 600-57-7 MP (°C):

MW: 330.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.333E-05	3.084E-02	37	C400	2 0 2 2 2	

4237. C₂₁H₃₀O₃

5,6-Dehydroisoandrosterone acetate

Androst-5-en-17-one, 3-(acetoxy)-, (3β)-

RN: 853-23-6 MP (°C): 166

MW: 330.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.480E-05	1.150E-02	ns	B057	0 2 1 1 2	

4238. C₂₁H₃₀O₃

Testosterone acetate

17-O-Acetyltestosterone

Androst-4-en-3-one, 17-(acetoxy)-, (17β)-

RN: 1045-69-8 MP (°C): 140

MW: 330.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.111E-06	2.350E-03	25	J004	1 0 1 1 2	
7.111E-06	2.350E-03	ns	B057	0 2 1 1 2	

4239. C₂₁H₃₀O₃17- α -Hydroxyprogesterone

Pregn-4-ene-3,20-dione, 17-hydroxy-

Prodix

Prodox

U 3096

RN: 68-96-2**MP (°C):** 222**MW:** 330.47**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E-05	5.056E-03	20	L077	1 2 2 2 2	
1.960E-05	6.477E-03	27.34	L077	1 2 2 2 2	
2.760E-05	9.121E-03	35	L077	1 2 2 2 2	
3.580E-05	1.183E-02	42.34	L077	1 2 2 2 2	
4.290E-05	1.418E-02	50	L077	1 2 2 2 2	

4240. C₂₁H₃₀O₄

Corticosterone

11,21-Dihydroxyprogesterone

8(4)-Pregnene-11 β ,21-diol-3,20-dione11 β ,21-Dihydroxypregn-4-ene-3,20-dione**RN:** 50-22-6 **MP (°C):** 182**MW:** 346.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.943E-04	2.405E-01	37	C400	2 0 2 2 2	

4241. C₂₁H₃₀O₄11 β ,17 α -Dihydroxy-4-pregnene-3,20-dione

Pregn-5-ene-3,20-dione, 11,17-dihydroxy-

Pregn-5-ene-3,20-dione, 11 β ,17-dihydroxy-**RN:** 603-97-4 **MP (°C):****MW:** 346.47 **BP (°C):** 516.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.361E-04	8.180E-02	37	C400	2 0 2 2 2	

4242. C₂₁H₃₀O₄

Cortexolone

11-Deoxy-17-hydroxycorticosterone

11-Deoxycortisol

11-Desoxycortisone

17,21-Dihydroxy-4-pregnene-3,20-dione

17 α ,21-Dihydroxypregn-4-ene-3,20-dione**RN:** 152-58-9 **MP (°C):** 208**MW:** 346.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.272E-04	4.408E-02	37	C400	2 0 2 2 2	

4243. C₂₁H₃₀O₅

Hydrocortisone

11 β ,17,21-Trihydroxypregn-4-ene-3,20-dione

Colifoam

Cortaid

Cortef

Bactine

RN: 50-23-7 **MP (°C):** 218.5**MW:** 362.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.780E-04	1.733E-01	10	B012	2 0 1 1 0	
7.725E-04	2.800E-01	20	A067	0 0 0 0 1	
7.430E-04	2.693E-01	20	B012	2 0 1 1 0	
8.109E-04	2.939E-01	22.5	B422	2 0 2 2 2	
8.820E-04	3.197E-01	25	B012	2 0 1 1 0	
9.932E-04	3.600E-01	25	C437	0 0 0 0 0	Average
7.725E-04	2.800E-01	25	H015	1 0 0 0 1	
8.194E-04	2.970E-01	25	H098	1 0 2 0 2	
8.190E-04	2.969E-01	25	H320	0 0 0 0 0	
8.194E-04	2.970E-01	25	H320	0 0 0 0 0	
7.860E-04	2.849E-01	25	K003	2 1 1 1 1	
1.614E-03	5.850E-01	25	K021	1 2 2 2 1	
7.725E-04	2.800E-01	25	M023	1 0 2 1 1	
9.896E-03	3.587E+00	25	P324	0 0 0 0 0	
1.034E-03	3.748E-01	30	B012	2 0 1 1 0	
1.000E-03	3.625E-01	30	L344	2 0 1 1 0	EFG
1.077E-03	3.905E-01	37	C400	2 0 2 2 2	
1.070E-03	3.878E-01	37	H036	1 0 2 2 2	EFG
1.265E-03	4.585E-01	40	B012	2 0 1 1 0	
1.519E-03	5.506E-01	50	B012	2 0 1 1 0	
7.725E-04	2.800E-01	298	F016	0 0 0 0 0	
1.159E-03	4.200E-01	amb	L434	0 0 0 0 0	
1.104E-03	4.000E-01	amb	L445	0 0 0 0 0	Intrinsic
7.116E-04	2.579E-01	ns	B404	0 2 1 1 0	

4244. C₂₁H₃₀O₆

Cortisone acetate

Pregn-4-ene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-

RN: 50-04-4 MP (°C): 235

MW: 378.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.284E-05	2.000E-02	22.5	G301	0 0 0 0 0	
5.020E-05	1.900E-02	25	K003	2 1 1 1 1	
5.284E-05	2.000E-02	25	M023	1 0 2 1 0	
7.398E-05	2.800E-02	25	P096	0 0 0 0 0	
1.000E-04	3.785E-02	30	L068	1 0 0 1 0	EFG

4245. C₂₁H₃₁NO

N-Cyclododecylcinnamamide

2-Propenamide, *N*-cyclododecyl-3-phenyl

RN: 59832-03-0 MP (°C):

MW: 313.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.910E-08	1.226E-05	ns	H350	0 0 0 0 0	

4246. C₂₁H₃₁N₃O₂2-Pentoxy-*N*-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide*N*-[2-(Diethylamino)ethyl]-2-pentoxyquinoline-4-carboxamide

RN: 2717-02-4 MP (°C):

MW: 357.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.300E-05	1.895E-02	ns	B018	0 0 0 0 1	
5.300E-05	1.895E-02	ns	M066	0 0 0 0 1	

4247. C₂₁H₃₂O₂

3,20-Pregnanedione

7 α -17-Dimethyltestosterone

Bolasterone

RN: 128-23-4 MP (°C):

MW: 316.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.833E-04	5.800E-02	37	H004	0 0 0 0 0	

4248. C₂₁H₃₂O₂7 α ,17-Dimethyl-19-nortestosterone**RN:** MP (°C):**MW:** 316.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.434E-04	4.540E-02	37	H004	0 0 0 0 0	

4249. C₂₁H₃₂O₂

Pregnenolone

3 β -Hydroxy-5-pregn-en-20-one5-Pregnen-3 β -ol-20-one3 β -Hydroxypregn-5-en-20-one**RN:** 145-13-1 MP (°C): 193**MW:** 316.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.230E-05	7.058E-03	37	H034	1 0 2 1 2	pH 7.4
9.479E-05	3.000E-02	amb	L434	0 0 0 0 0	
1.295E-04	4.100E-02	rt	B408	0 0 2 2 2	

4250. C₂₁H₃₂O₃

Androstanolone acetate

Androstan-3-one, 17-(acetoxy)-, (5 α ,17 β)-

Stanalone acetate

RN: 1164-91-6 MP (°C):**MW:** 332.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.672E-01	8.884E+01	ns	B057	0 2 1 1 2	

4251. C₂₁H₃₃NO2-Propenamide, *N*-dodecyl-3-phenyl-**RN:** 55125-24-1 MP (°C):**MW:** 315.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-06	6.626E-04	ns	H350	0 0 0 0 0	

4252. C₂₁H₃₃NO₇

Lasiocarpine

(7 α -Angelyloxy-5,6,7,8 α -tetrahydro-3H-pyrrolizin-1-yl)methyl-2,3-dihydroxy-2-(1'-methoxyethyl)-3-methylbutyrate

RN: 303-34-4 MP (°C): 97

MW: 411.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.641E-02	6.754E+00	ns	I312	0 0 0 0 0	

4253. C₂₁H₃₄O₂

Pregnanolone

3-Deoxo-3 α -hydroxy-5 β -dihydroprogesterone3 α ,5 β -Tetrahydroprogesterone3 α -Hydroxy-5 β -pregnan-20-onePregnan-3 α -ol-20-one3 α ,5 β -Pregnanolone

RN: 128-20-1 MP (°C):

MW: 318.50 BP (°C): 431.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.512E-05	8.000E-03	rt	B408	0 0 2 2 2	

4254. C₂₁H₃₄O₃Tetradecyl *p*-hydroxybenzoate

Tetradecyl 4-hydroxybenzoate

RN: 71177-53-2 MP (°C):

MW: 334.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.088E-03	3.639E-01	25	D081	1 2 2 1 2	

4255. C₂₁H₃₅NO₃

4-Octoxybenzoic acid-2-(diethyl-amino)ethyl ester

RN: 38973-76-1 MP (°C):

MW: 349.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.398E-02	ns	M066	0 0 0 0 1	

4256. C₂₁H₃₆O₄

4-Nonylphenol triethoxylate

Ethanol, 2-[2-[2-(4-nonylphenoxy)ethoxy]ethoxy]-

RN: 51437-95-7 MP (°C):

MW: 352.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.668E-05	5.880E-03	20.5	A335	0 0 0 0 0	
1.670E-05	5.887E-03	20.5	A335	0 0 0 0 0	

4257. C₂₁H₄₀O₄

α-Monoolein

1-Monoolein

Glycerol monooleate

9-Octadecenoic acid (Z)-, monoester with 1,2,3-propanetriol

1-Oleoyl-sn-glycerol

RN: 25496-72-4 MP (°C):

MW: 356.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<3.57E-03	30	O321	0 0 0 0 0	

4258. C₂₁H₄₄

3-Methyleicosane

18-Methyleicosane

RN: 6418-46-8 MP (°C):

MW: 296.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.294E-13	1.570E-10	23	C332	0 0 0 0 0	

4259. C₂₁H₄₄

2-Methyleicosane

19-Methyleicosane

RN: 1560-84-5 MP (°C):

MW: 296.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.091E-13	1.510E-10	23	C332	0 0 0 0 0	

4260. C₂₂H₁₂

Indeno(1,2,3-cd)pyrene

Indeno[1,2,3-cd]pyrene

o-Phenylenepyrene

RN: 193-39-5 **MP (°C):** 162.5
MW: 276.34 **BP (°C):** 536

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.876E-10	1.900E-07	ns	W302	0 0 0 0 1	

4261. C₂₂H₁₂

Benzo[g,h,i]perylene

Benz[g,h,i]perylene

RN: 191-24-2 **MP (°C):** 279
MW: 276.34 **BP (°C):** >500

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.958E-10	1.370E-07	25	D406	1 2 2 2 2	
6.500E-10	1.796E-07	25	K123	1 0 2 2 1	
9.409E-10	2.600E-07	25	M064	1 1 2 2 1	
9.400E-10	2.598E-07	25	M342	1 0 1 1 1	
9.409E-10	2.600E-07	ns	M344	0 0 0 0 1	
2.533E-09	7.000E-07	ns	W302	0 0 0 0 0	

4262. C₂₂H₁₄

Picene

1,2,7,8-Dibenzphenanthrene

3,4-Benzchrysene

RN: 213-46-7 **MP (°C):** 366
MW: 278.36 **BP (°C):** 518

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.550E-08	4.315E-06	20	E009	1 0 0 1 2	
8.981E-09	2.500E-06	27	D003	1 0 0 1 1	

4263. C₂₂H₁₄

1,2,3,4-Dibenzanthracene

RN: 215-58-7 **MP (°C):** 205
MW: 278.36 **BP (°C):** 518

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.748E-09	1.600E-06	25	B319	2 0 1 2 1	
8.200E-08	2.283E-05	25	K123	1 0 2 2 1	

4264. C₂₂H₁₄

1,2:7,8-Dibenzanthracene

Dibenz[a,j]anthracene

Dinaphthalanthracene

RN: 224-41-9 MP (°C): 196

MW: 278.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.100E-08	8.629E-06	25	K123	1 0 2 2 1	
4.311E-08	1.200E-05	27	D003	1 0 0 1 1	

4265. C₂₂H₁₄

1,2:5,6-Dibenzanthracene

1,2,5,6-Dibenzanthracene

RN: 53-70-3 MP (°C): 266

MW: 278.36 BP (°C): 524

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.945E-09	2.490E-06	24	H106	1 0 2 2 2	
7.904E-09	2.200E-06	25	B319	2 0 1 2 2	
2.150E-09	5.985E-07	25	K001	2 2 2 2 2	
1.100E-07	3.062E-05	25	K123	1 0 2 2 1	sic
8.945E-09	2.490E-06	25	M156	1 2 1 1 2	
1.800E-09	5.010E-07	25	M342	1 0 1 1 2	
1.796E-09	5.000E-07	27	D003	1 0 0 1 1	

4266. C₂₂H₁₆F₃N₃

Fluotrimazole

1H-1,2,3-Triazole, 1-[diphenyl[3-(trifluoromethyl)phenyl]methyl]-

RN: 57381-79-0 MP (°C): 132

MW: 379.39 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.954E-09	1.500E-06	20	M161	1 0 0 0 1	

4267. C₂₂H₁₆O₈

Ethyl biscoumacetate

Tromexan

RN: 548-00-5 MP (°C): 154

MW: 408.37 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.179E-04	8.900E-02	20	K028	2 1 2 1 2	pH 3.8, form I
3.747E-04	1.530E-01	20	K028	2 1 2 1 2	pH 3.8, form II
2.179E-04	8.899E-02	20	M042	1 0 0 0 1	pH 3.8, form I, mp 172-182 C
3.761E-04	1.536E-01	20	M042	1 0 0 0 2	pH 3.8, form II, mp 153-160 C

4268. C₂₂H₁₇ClN₂

Clotrimazole

1-(*o*-Chloro- α , α -diphenylbenzyl)imidazole1-[α -(2-Chlorophenyl)benzhydryl]imidazole

Lotrimin

RN: 23593-75-1 MP (°C): 147–149

MW: 344.85 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.90E-05	<1.00E-02	25	H328	0 0 0 0 0	
8.700E-05	3.000E-02	amb	L434	0 0 0 0 0	

4269. C₂₂H₁₈N₂O₄SHydantoin, 5,5-diphenyl-1-(*o*-tolylsulfonyl)-1-(*o*-Methylbenzenesulfonyl)-5,5-diphenyl-hydantoin

RN: 24759-41-9 MP (°C):

MW: 406.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.870E-06	7.600E-04	37	F183	1 0 1 1 2	intrinsic

4270. C₂₂H₁₈N₂O₅S1-(*p*-Methoxylbenzenesulfonyl)-5,5-diphenyl-hydantoin

RN: 24759-37-3 MP (°C):

MW: 422.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.207E-06	5.100E-04	37	F183	1 0 1 1 2	intrinsic

4271. C₂₂H₁₉Br₂NO₃

Deltamethrin

3-(2,2-Dibromoethyl)-2,2-dimethylcyclopropanecarboxylic acid, cyano(3-phenoxyphenyl)methyl ester

RN: 52918-63-5 MP (°C): 98–101

MW: 505.22 BP (°C): 300

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.959E-09	2.000E-06	25	M364	1 0 0 0 1	
3.959E-09	2.000E-06	ns	V414	0 0 0 0 0	

4272. C₂₂H₁₉F₆NOS α -Piperidyl-3,6-bis(trifluoromethyl)-9-phenanthrenemethanol

RN: 31817-24-0 MP (°C): 215

MW: 459.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.632E-05	7.500E-03	25	A013	1 0 2 2 0	average

4273. C₂₂H₂₀

10-Butyl-1,2-benzanthracene

RN: 188124-94-9 MP (°C): 97

MW: 284.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.813E-08	8.000E-06	27	D003	1 0 0 1 1	

4274. C₂₂H₂₀Cl₂N₂O₃

Benzofenap

2-((4-(2,4-Dichloro-3-methylbenzoyl)-1,3-dimethyl-1H-pyrazol-5-yl)oxy)-1-(4-methylphenyl) ethanone

RN: 82692-44-2 MP (°C):

MW: 431.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.020E-07	1.303E-04	ns	R427	0 0 0 0 0	

4275. C₂₂H₂₀O₁₃

Carminic acid

Carmine

Carminsaeure

RN: 1260-17-9 MP (°C):

MW: 492.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.637E-03	1.298E+00	rt	D021	0 0 1 1 1	

4276. C₂₂H₂₂ClN₃O₅

Propaquizafop

2-[Isopropylideneamino]oxyethyl (*R*)-2-[*p*-[(6-chloro-2-quinoxalinyloxy)phenoxy]-propionate
(R)-2-{[(1-Methylethylidene)amino]oxy}ethyl 2-{4-[(6-chloro-2-quinoxalinyloxy)phenoxy]propanoate}

Agil

Shogun

RO 17-3664

RN: 111479-05-1 **MP (°C):****MW:** 443.89 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.413E-06	6.270E-04	ns	R427	0 0 0 0 0	

4277. C₂₂H₂₂FN₃O₂

Droperidol

2H-Benzimidazol-2-one, 1-[1-[4-(4-fluorophenyl)-4-oxobutyl]-1,2,3,6-tetrahydro-4-pyridinyl]-1,3-dihydro-

Sintodril

Neurolidol

R 4749

RN: 548-73-2 **MP (°C):****MW:** 379.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.081E-05	4.100E-03	30	P044	0 0 0 0 0	

4278. C₂₂H₂₂N₂O₄*N,N'*-Dibutyl-1,4,5,8-naphthalenediimide

Benzol[*lmn*][3,8]phenanthroline-1,3,6,8(2H,7H)-tetrone, 2,7-dibutyl-1,4,5,8-Naphthalenetetracarboxylic 1,8:4,5-diimide, *N,N'*-dibutyl-

RN: 17655-95-7 **MP (°C):****MW:** 378.43 **BP (°C):** 572.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-09	1.892E-06	23	B410	2 1 2 2 2	

4279. C₂₂H₂₂N₂O₈

Methacycline base

Oxytetracycline, 6-methylene-

Tri-methacycline

Rondomycin

RN: 914-00-1

MP (°C):

MW: 442.43

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.706E-02	7.548E+00	21	M044	2 0 2 2 2	

4280. C₂₂H₂₂N₄O₆

Benzoyl-mitomycin C

RN: 438.44 MP (°C):

MW: 438.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	4.384E-03	25	M316	1 1 1 1 2	

4281. C₂₂H₂₃CIN₂O₈

Chlortetracycline

7-Chlortetracycline

Acronize PD

Acronize

RN: 57-62-5 MP (°C):

MW: 478.89 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.316E-03	6.300E-01	25	B191	1 0 0 0 1	
2.297E-03	1.100E+00	37	M104	1 2 1 1 0	form II, EFG, recrystallized
1.566E-03	7.500E-01	37	M104	1 2 1 1 0	form I, EFG, recrystallized
2.088E-04	1.000E-01	37	M105	1 2 1 1 0	EFG

4282. C₂₂H₂₃NO₃

Fenpropane

Danitol

Herald

WL 41706

Miothrin

2,2,3,3-Tetramethylcyclopropane carboxylic acid, cyano(3-phenoxyphenyl)methyl ester

RN: 39515-41-8 **MP (°C):****MW:** 349.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.074E-08	1.424E-05	ns	R427	0 0 0 0 0	

4283. C₂₂H₂₃NO₇

Noscapine

Narcotine

O-Methylnarcotoline

Opianin

Opian

RN: 128-62-1 **MP (°C):** 176**MW:** 413.43 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-05	1.654E-02	15	K059	2 2 2 0 0	
7.327E-04	3.029E-01	25	D004	0 0 0 0 0	
7.256E-04	3.000E-01	30	A073	1 1 1 1 0	
1.693E-03	7.000E-01	40	A073	1 1 1 1 0	
2.419E-03	1.000E+00	50	A073	1 1 1 1 1	
2.419E-03	1.000E+00	60	A073	1 1 1 1 1	
2.419E-03	1.000E+00	70	A073	1 1 1 1 1	
2.419E-03	1.000E+00	80	A073	1 1 1 1 1	
3.628E-03	1.500E+00	90	A073	1 1 1 1 1	
4.838E-03	2.000E+00	100	A073	1 1 1 1 1	

4284. C₂₂H₂₄ClN₅O₂

Domperidone

5-Chloro-1-[1-[3-(2-oxo-1-benzimidazolinyl)propyl]-4-piperidyl]-2-benzimidazolinone

RN: 57808-66-9 **MP (°C):** 242.5**MW:** 425.92 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.015E-05	1.710E-02	22	J420	0 0 0 0 0	pH6.5

4285. C₂₂H₂₄N₂O₈

Tetracycline
Achromycin V
Sumycin
Robitet
Panmycin

RN: 60-54-8 **MP (°C):** 176dec
MW: 444.45 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.900E-04	4.400E-01	25	B191	1 0 0 0 1	neutral pH
5.200E-04	2.311E-01	25	G012	2 0 2 1 0	EFG, pH 5.0
5.700E-04	2.533E-01	25	H017	1 2 2 2 0	EFG, pH 5.0
2.655E-03	1.180E+00	29	N031	1 2 2 2 0	EFG, pH 5.0
7.600E-04	3.378E-01	30	L069	1 0 1 1 0	EFG
1.777E-03	7.900E-01	35	N031	1 2 2 2 0	EFG, pH 5.0
7.875E-02	3.500E+01	37	M104	1 2 1 1 2	form II, recrystallized
6.232E-02	2.770E+01	37	M104	1 2 1 1 2	form I, recrystallized
6.478E-04	2.879E-01	ns	N302	0 2 1 2 2	

4286. C₂₂H₂₄N₂O₈.H₂O

Doxycycline (monohydrate)
Doxylin
Monodox
Vibra-tabs
Doxycaps
Vibramycin

RN: 564-25-0 **MP (°C):** 201dec
MW: 462.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.362E-03	6.300E-01	25	B132	2 1 1 1 0	EFG

4287. C₂₂H₂₄N₂O₉

Oxytetracycline
Glomycin
Hydroxytetracycline
Riomitsin
Terrafungine
Stevacin

RN: 79-57-2 **MP (°C):** 184
MW: 460.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.234E-04	1.950E-01	20	L051	1 0 0 0 2	
9.990E-04	4.600E-01	25	B191	1 0 0 0 1	neutral pH <i>(continued)</i>

4287. C₂₂H₂₄N₂O₉ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.800E-04	2.210E-01	25	G012	2 0 2 1 0	EFG, pH 5.0
6.798E-04	3.130E-01	25	H005	1 0 1 2 2	Ph 5.8
5.000E-04	2.302E-01	25	H017	1 2 2 2 0	EFG, pH 5.0
6.515E-04	3.000E-01	29	N031	1 2 2 2 0	EFG, pH 5.0
8.687E-04	4.000E-01	37	M104	1 2 1 1 0	form II, EFG, recrystallized
6.515E-04	3.000E-01	37	M104	1 2 1 1 0	form I, EFG, recrystallized

4288. C₂₂H₂₄N₄O₅

Benzyl-mitomycin C

RN: MP (°C):
 MW: 424.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-03	6.324E-01	25	M316	1 1 1 1 2	

4289. C₂₂H₂₄N₄O₅SMethanesulfonamide, *N*-[1'-[2-(2,1,3-benzoxadiazol-5-yl)ethyl]-3,4-dihydro-4-oxospiro[2H-1-benzopyran-2,4'-piperidin]-6-yl]-Methanesulfonamide, *N*-[1'-[2-(5-benzofurazanyl)ethyl]-3,4-dihydro-4-oxospiro[2H-1-benzopyran-2,4'-piperidin]-6-yl]-

RN: MP (°C):
 MW: 456.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.752E-05	8.000E-03	22	D405	1 1 2 2 2	Intrinsic

4290. C₂₂H₂₅NO₆

Colchicine

Colchicin

RN: 64-86-8 MP (°C):
 MW: 399.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.629E-02	3.846E+01	20	D041	1 0 0 0 0	
1.088E-01	4.348E+01	25	D004	0 0 0 0 0	
8.261E-02	3.300E+01	ns	K444	0 0 0 0 0	

4291. C₂₂H₂₆F₃N₃OS

Fluphenazine

Permitil

Modecate

Prolixin

RN: 69-23-8 **MP (°C):** <25**MW:** 437.53 **BP (°C):** 271

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.100E-05	3.106E-02	37	F011	1 0 1 1 1	pH 7.4

4292. C₂₂H₂₆N₂O₉

Doxycycline

4-(Dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-2-naphthacenecarboxamide monohydrate

Doryx

Doxylin

Monodox

Vibramycin

RN: 564-25-0 **MP (°C):****MW:** 462.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.350E+00	1.087E+03	25	B443	0 0 0 0 0	
2.162E-04	1.000E-01	ns	K444	0 0 0 0 0	

4293. C₂₂H₂₇CIN₂O₄S

Diltiazem hydrochloride

1,5-Benzothiazepin-4(5H)one,3-(acetoxy)-5-(2-(dimethylamino)ethyl)-2,3-dihydro-2-(4-methoxyphenyl)-,

Dilacor XR

Cardizem

Cardcal

Coras

RN: 33286-22-5 **MP (°C):****MW:** 450.99 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.131E-03	5.100E-01	25	A412	1 0 2 2 1	int

4294. C₂₂H₂₇NO₂

Danazol

17 α -Pregna-2,4-dien-20-yne[2,3-d]isoxazol-17-ol

Danocrine

Cyclomen

RN: 17230-88-5 MP (°C):

MW: 337.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.719E-06	5.800E-04	25	E409	0 0 0 0 0	
1.245E-06	4.200E-04	37	S446	0 0 0 0 0	

4295. C₂₂H₂₈F₂O₅

Flumethasone

Flumethasonipivalate

RN: 2135-17-3 MP (°C):

MW: 410.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.436E-06	1.000E-03	20	A067	0 0 0 0 0	

4296. C₂₂H₂₈N₂O

Fentanyl

1-Phenethyl-4-(phenylpropionylamino)piperidine

N-(1-Phenethyl-4-piperidyl)propionanilide

Duragesic

RN: 437-38-7 MP (°C):

MW: 336.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.944E-04	2.000E-01	25	R338	0 0 0 0 0	
3.566E-05	1.200E-02	35	R418	0 0 0 0 0	Intrinsic

4297. C₂₂H₂₈N₆O₃S

Delavirdine

1-[3-[(1-Methylethyl)amino]-2-pyridinyl]-4-[[5-[(methylsulfonyl)amino]-1H-indol-2-yl]carbonyl]piperazine

1-(5-Methanesulfonamido-1H-indol-2-ylcarbonyl)-4-[3-(1-methylethylamino)pyridinyl]piperazine

1-[3-(Isopropylamino)-2-pyridyl]-4-[(5-methanesulfonamidoindol-2-yl)carbonyl]piperazine

RN: 136817-59-9 MP (°C):

MW: 456.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.571E-02	3.000E+01	ns	A426	0 0 0 0 0	Intrinsic

4298. C₂₂H₂₈O₃

Canrenone

17-Hydroxy-3-oxo-17α-pregna-4,6-diene-21-carboxylic acid lactone

RN: 976-71-6 MP (°C): 149-151

MW: 340.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-07	2.724E-04	25	G017	1 0 1 0 0	EFG
8.100E-05	2.758E-02	37	C004	0 0 0 0 0	<i>sic</i>
8.958E-07	3.050E-04	37	O306	1 0 2 2 2	
6.374E-07	2.170E-04	rt	O306	0 0 2 2 2	

4299. C₂₂H₂₈O₃

Norethindrone acetate

Norethisterone acetate

RN: 51-98-9 MP (°C): 161

MW: 340.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.288E-06	3.162E-03	10	L078	1 0 1 2 0	EFG
1.312E-05	4.467E-03	20	L078	1 0 1 2 0	EFG
1.570E-05	5.345E-03	25	H099	1 0 2 2 2	
1.652E-05	5.623E-03	25	L078	1 0 1 2 2	
1.853E-05	6.310E-03	30	L078	1 0 1 2 0	EFG
2.937E-05	1.000E-02	40	L078	1 0 1 2 0	EFG

4300. C₂₂H₂₉FO₄

Fluorometholone

9-Fluoro-11β,17-dihydroxy-6α-methylpregna-1,4-diene-3,20-dione

21-Desoxy-9α-fluoro-6α-methyl-prednisolone

RN: 426-13-1 MP (°C):

MW: 376.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.968E-05	3.000E-02	25	G008	1 2 1 1 0	

4301. C₂₂H₂₉FO₅

Betamethasone

Pregna-1,4-diene-3,20-dione, 9-fluoro-11,17,21-trihydroxy-16-methyl-, (11β,16β)-

RN: 378-44-9 MP (°C): 230

MW: 392.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.478E-04	5.800E-02	25	K003	2 1 1 1 1	
1.936E-04	7.599E-02	25	P096	0 0 0 0 0	

(continued)

4301. C₂₂H₂₉FO₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.500E-04	5.887E-02	30	O321	0 0 0 0 0	
1.529E-04	6.000E-02	30	O321	0 0 0 0 0	
1.605E-04	6.301E-02	37	C400	2 0 2 2 2	
1.605E-04	6.300E-02	ns	B404	0 2 1 1 0	
1.575E-04	6.180E-02	rt	I404	0 0 0 0 0	Intrinsic, Average

4302. C₂₂H₂₉FO₅

Dexamethasone

Dexamethasone alcohol

RN: 50-02-2 MP (°C): 262
 MW: 392.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.200E-05	3.218E-02	10	B012	2 0 1 1 0	
1.580E-04	6.201E-02	20	B012	2 0 1 1 0	
2.800E-04	1.099E-01	23	L345	1 0 1 1 2	
2.270E-04	8.909E-02	25	B012	2 0 1 1 0	
2.140E-04	8.399E-02	25	K003	2 1 1 1 1	
3.083E-04	1.210E-01	25	K021	1 2 2 2 1	
2.548E-04	1.000E-01	25	P312	0 0 0 0 0	
2.520E-04	9.890E-02	30	B012	2 0 1 1 0	
2.344E-04	9.200E-02	37	C400	2 0 2 2 2	
2.955E-04	1.160E-01	37	D026	0 0 0 0 0	
3.560E-04	1.397E-01	40	B012	2 0 1 1 0	
4.600E-04	1.805E-01	50	B012	2 0 1 1 0	
4.077E-04	1.600E-01	amb	L434	0 0 0 0 0	
2.548E-04	1.000E-01	ns	K444	0 0 0 0 0	
1.707E-04	6.700E-02	ns	N302	0 2 1 2 1	

4303. C₂₂H₂₉NO₇S₂Methyl O-acetyl-3-(acetoxy)-N-{5-[*(3R*)-1,2-dithiolan-3-yl]-pentanoyl}-L-tyrosinate

RN: MP (°C):
 MW: 483.61 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.817E-04	2.329E-01	ns	S453	0 0 0 0 0	

4304. C₂₂H₃₀ClNO₂

Propoxyphene hydrochloride

D-Propoxyphene hydrochloride

RN: 1639-60-7 MP (°C):

MW: 375.94 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.842E-06	3.700E-03	25	A412	1 0 2 2 1	int

4305. C₂₂H₃₀Cl₂N₁₀

Chlorhexidin

Chlorhexidine

bis(5-(*p*-Chlorophenyl)biguanidinio)hexane

RN: 55-56-1 MP (°C):

MW: 505.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.583E-04	7.999E-02	20	D341	0 0 0 0 0	
8.309E-05	4.200E-02	22.5	G301	0 0 0 0 0	

4306. C₂₂H₃₀N₂O₂

Aspidospermine

Aspidospermidine, 1-acetyl-17-methoxy-

RN: 466-49-9 MP (°C): 208

MW: 354.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.701E-04	1.666E-01	c	D004	0 0 0 0 0	

4307. C₂₂H₃₀N₂O₂S

Sufentanil

N-[4-(Methoxymethyl)-1-[2-(2-thienyl)ethyl]-4-piperidyl]propionanilide

Sufenta

RN: 56030-54-7 MP (°C):

MW: 386.56 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.966E-04	7.600E-02	25	R338	0 0 0 0 0	
3.363E-06	1.300E-03	35	R418	0 0 0 0 0	Intrinsic

4308. C₂₂H₃₀O₅

Methylprednisolone

6 α -Methylprednisolone

Medrol

Solumedrol

Metrisone

Promacortine

RN: 83-43-2**MP (°C):** 232.5**MW:** 374.48**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.204E-04	1.200E-01	25	A014	1 0 1 1 0	EFG
2.403E-04	9.000E-02	25	A014	1 0 1 1 0	EFG, pH 5.0
2.534E-03	9.491E-01	25	G008	1 2 1 1 1	
3.445E-04	1.290E-01	25	K021	1 2 2 2 1	
1.335E-04	5.000E-02	27.14	H026	1 0 2 1 0	EFG, form I
1.923E-04	7.199E-02	30.0	H010	2 2 1 1 1	
4.273E-04	1.600E-01	31.72	H026	1 0 2 1 0	EFG, form II
3.124E-04	1.170E-01	37	H004	0 0 0 0 0	polymorph I
3.765E-04	1.410E-01	37	H004	0 0 0 0 0	polymorph II
5.341E-04	2.000E-01	40.32	H026	1 0 2 1 0	EFG, form II
2.937E-04	1.100E-01	40.32	H026	1 0 2 1 0	EFG, form I
4.273E-04	1.600E-01	51.52	H026	1 0 2 1 0	EFG, form I
1.362E-03	5.100E-01	81.45	H026	1 0 2 1 0	EFG, form II
1.068E-03	4.000E-01	81.45	H026	1 0 2 1 0	EFG, form I
2.670E-04	1.000E-01	ns	M169	0 0 0 0 1	

4309. C₂₂H₃₀O₆5,16- β -Dihydroxy-6- β -methyl-3,11-dioxo-5- α -pregn-17(20)-ene-*cis*-20-carboxylic acid methyl ester

U-20235

RN: MP (°C):**MW:** 390.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.402E-04	2.500E-01	ns	K029	0 0 2 1 1	

4310. C₂₂H₃₂O₃

Nandrolone butyrate

RN: MP (°C):**MW:** 344.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.460E-05	5.030E-03	37	C026	0 0 0 0 0	

4311. C₂₂H₃₂O₃

Methyltestosterone acetate

17- α -Methyltestosterone acetate

RN: 1099-79-2 **MP (°C):** 164
MW: 344.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.430E-05	4.926E-03	25	H099	1 0 2 2 2	
5.196E-06	1.790E-03	ns	B057	0 2 1 1 2	

4312. C₂₂H₃₂O₃

5,6-Dehydroisoandrosterone propionate

RN: 1167-87-9 **MP (°C):**
MW: 344.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.415E-05	8.320E-03	ns	B057	0 2 1 1 2	

4313. C₂₂H₃₂O₃

Testosterone propionate

17-(1-Oxopropoxy)-(17 β)-androst-4-en-3-one

Testosterone-17-propionate

Agovirin

Androsan

Androgen

RN: 57-85-2 **MP (°C):** 120
MW: 344.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.710E-04	5.891E-02	20	F012	1 0 1 1 1	
4.300E-06	1.481E-03	25	J004	1 0 1 1 2	
5.806E-06	2.000E-03	25	K003	2 1 1 1 1	
6.096E-06	2.100E-03	30	T005	2 0 2 2 1	
1.060E-05	3.652E-03	37.50	B054	1 0 1 1 2	
4.296E-06	1.480E-03	ns	B057	0 2 1 1 2	

4314. C₂₂H₃₃N₃O₂

2-Hexoxy-N-[2-(diethyl-amino)ethyl]-4-quinoline carboxamide

N-[2-(Diethylamino)ethyl]-2-hexoxyquinoline-4-carboxamide

RN: 2717-03-5 **MP (°C):**
MW: 371.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.700E-06	2.489E-03	ns	B018	0 0 0 0 1	
6.700E-06	2.489E-03	ns	M066	0 0 0 0 1	

4315. C₂₂H₃₄Cl₂O₃2,4-Dichlorophenoxyacetic acid *n*-tetradecyl ester

RN: 65267-96-1 **MP (°C):**
MW: 417.42 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.161E-05	4.848E-03	ns	M120	0 0 1 1 2	

4316. C₂₂H₃₄N₆O₄

2,5-Diaziridinyl-3,6-di(1'-piperazineethanol)-1,4-benzoquinone

RN: 59886-40-7 **MP (°C):** 170
MW: 446.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.479E-02	2.000E+01	rt	C317	0 0 0 0 0	

4317. C₂₂H₃₄O₃

Androstanolone propionate

Androstan-3-one, 17-(1-oxopropoxy)-, (5 α ,17 β)-

RN: 855-22-1 **MP (°C):**
MW: 346.51 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.789E-06	6.200E-04	ns	B057	0 2 1 1 2	

4318. C₂₂H₃₅NO₃

Acetaminophen myristate

Acetaminophen tetradecanoate

RN: 54942-39-1 **MP (°C):** 114
MW: 361.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.660E-05	6.000E-03	25	B010	1 1 1 1 0	

4319. C₂₂H₃₇NO₂

Anandamide

Arachidonoylethanolamide

AEA

RN: 94421-68-8 **MP (°C):**
MW: 347.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.188E-06	4.130E-04	25	J414	0 0 0 0 0	Intrinsic

4320. C₂₂H₃₈O₅

4-Octylphenol tetraethoxylate

Ethanol, 2-[2-[2-(4-octylphenoxy)ethoxy]ethoxy]-

RN: 51437-92-4 **MP (°C):****MW:** 382.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.404E-05	2.450E-02	20.5	A335	0 0 0 0 0	
6.410E-05	2.452E-02	20.5	A335	0 0 0 0 0	

4321. C₂₂H₃₉O₃P

Diisooctyl phenyl phosphonate

RN: **MP (°C):****MW:** 382.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.61E-04	<1.00E-01	25	B070	1 2 0 1 0	

4322. C₂₂H₃₉O₃P

Diocetyl phenyl phosphonate

Di-n-octyl phenylphosphonate

DOPP

RN: 1754-47-8 **MP (°C):****MW:** 382.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.23E-04	<2.00E-01	25	B070	1 2 0 1 0	

4323. C₂₂H₄₂O₄

Diocetyl adipate

bis(2-Ethylhexyl) adipate

RN: 103-23-1 **MP (°C):****MW:** 370.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.095E-06	3.000E-03	25	F067	1 0 2 2 1	

4324. C₂₂H₄₃N₅O₁₃

Amikacin

Antibiotic BB-K8

RN: 37517-28-5 **MP (°C):** 203**MW:** 585.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.159E-01	1.850E+02	25	K044	1 0 0 0 2	pH 10.4

4325. C₂₃H₁₆O₆

Pamoic acid

4,4'-Methylenebis[3-hydroxy-2-naphthalenecarboxylic acid]

3,3'-Dihydroxy-4,4'-methylenedi-2-naphthoic acid

Embonic acid

RN: 130-85-8 MP (°C):

MW: 388.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-01	1.087E+02	ns	F007	0 0 0 0 1	

4326. C₂₃H₁₈F₂N₄O

α-(2,4-Difluorophenyl)-α-(1-2-(2-pyridyl)phenylethenyl)-1H-1,2,4-triazole-1-ethanol

XD405

RN: 124669-93-8 MP (°C):

MW: 404.42 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.418E-06	3.000E-03	22	M372	1 2 1 1 1	intrinsic

4327. C₂₃H₂₀N₂O₂S

G-1

p-Phenylthioethylphenylbutazone

1,2-Diphenyl-4-(2-phenylthioethyl)-3,5-pyrazolidinedione

RN: 3736-92-3 MP (°C):

MW: 388.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.118E-03	1.600E+00	ns	B158	0 0 0 0 1	pH 7.0

4328. C₂₃H₂₀N₂O₃S

Sulfinpyrazone

Sulfoxypyphenyl pyrazolidine

Sulfinpyrazole

1,2-Diphenyl-4-(2-(phenylsulfinyl)ethyl)-3,5-pyrazolidinedione

Anturane

RN: 57-96-5 MP (°C):

MW: 404.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.431E-03	2.601E+00	22	J420	0 0 0 0 0	pH6.5

4329. C₂₃H₂₂

10-Amyl-1,2-benzanthracene

RN: 188124-96-1 MP (°C):

MW: 298.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.681E-09	8.000E-07	27	D003	1 0 0 1 0	

4330. C₂₃H₂₂O₆

Rotenone

Tubatoxin

Derris

1,2,12,12α-Tetrahydro-2α-isopropenyl-8,9-dimethoxy(1)benzopyrano(3,4-b)furo(2,3-h)(1)
benzopyran-6(6α H)-one

RN: 83-79-4 MP (°C): 163

MW: 394.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.310E-07	1.700E-04	25	C100	1 0 2 1 1	
3.803E-05	1.500E-02	100	M161	1 0 0 0 1	

4331. C₂₃H₂₃NO

Trifemorph

Frescon

N-Tritylmorpholine

RN: 1420-06-0 MP (°C): 175

MW: 329.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.071E-08	2.000E-05	20	M161	1 0 0 0 1	

4332. C₂₃H₂₄N₄O₂

Diantipyrylmethane

4,4'-Methylenediantipyrine

4,4'-Diantipyrylmethane

RN: 1251-85-0 MP (°C): 182

MW: 388.47 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.130E-03	4.390E-01	20	P054	0 0 0 0 0	
1.132E-03	4.398E-01	20	P054	0 0 0 0 0	

4333. C₂₃H₂₄N₄O₆

Benzylcarbonyl-mitomycin C

RN: **MP (°C):**
MW: 452.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-03	1.014E+00	25	M316	1 1 1 1 2	

4334. C₂₃H₂₄N₄O₇

Benzoyloxycarbonyl-mitomycin C

RN: **MP (°C):**
MW: 468.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.200E-04	2.436E-01	25	M316	1 1 1 1 2	

4335. C₂₃H₂₄N₄S₂

Dithiodiantipyrynylmethane

3H-Pyrazole-3-thione, 4,4'-methylenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-

RN: 53799-78-3 **MP (°C):** 166
MW: 420.60 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	2.103E-01	ns	D087	0 2 0 0 1	

4336. C₂₃H₂₅N

Fendiline

RN: 13042-18-7 **MP (°C):**
MW: 315.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.389E-06	2.331E-03	22.5	B440	0 0 0 0 0	

4337. C₂₃H₂₆FN₃O₂

Spiperone

8-[4-(4-Fluorophenyl)-4-oxobutyl]-1-phenyl-1,3,8-triazaspiro[4.5]decan-4-one

RN: 749-02-0 **MP (°C):** 192 C
MW: 395.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.091E-05	3.200E-02	22	J420	0 0 0 0 0	pH6.5

4338. C₂₃H₂₆N₂O₄

Brucine

Brucin

RN: 357-57-3 **MP (°C):** 178
MW: 394.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.112E-03	3.200E+00	15	F300	1 0 0 0 1	
1.330E-03	5.247E-01	15	K059	2 2 2 0 2	
1.698E-02	6.700E+00	100	F300	1 0 0 0 1	
1.267E-03	4.998E-01	rt	D021	0 0 1 1 1	

4339. C₂₃H₂₆N₂O₄.4H₂O

Brucine (tetrahydrate)

Strychnidin-10-one, 2,3-dimethoxy-, tetrahydrate

RN: 5892-11-5 **MP (°C):** 105
MW: 466.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.677E-03	3.115E+00	c	D004	0 0 0 0 0	
1.420E-02	6.623E+00	h	D004	0 0 0 0 0	

4340. C₂₃H₂₆O₃

Phenothrin

(3-Phenoxyphenyl)methyl 2,2-dimethyl-3-(2-methyl-1-propenyl)cyclopropanecarboxylate

Sumithrin

3-Phenoxybenzyl D-*cis* and *trans*-2,2-dimethyl-3-(2-methylpropenyl)cyclopropanecarboxylate

RN: 26002-80-2 **MP (°C):** <25
MW: 350.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.707E-06	2.000E-03	30	M161	1 0 0 0 0	

4341. C₂₃H₂₇ClO₄

Delmadinone acetate

Pregna-1,4,6-triene-3,20-dione, 17-(acetoxy)-6-chloro-

RN: 13698-49-2 **MP (°C):** 168
MW: 402.92 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.506E-05	6.070E-03	37	K070	1 0 0 1 2	
1.134E-05	4.570E-03	ns	K070	1 0 0 1 2	

4342. C₂₃H₂₇FN₄O₂

Risperidal

3-(2-(4-(6-Fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl)ethyl)-6,7,8,9-tetrahydro-2-methyl-4H-pyrido[1,2-a]pyrimidin-4-one

Risperidone

RN: 106266-06-2 **MP (°C):****MW:** 410.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.090E-04	4.474E-02	25	E406	0 0 0 0 0	
<2.44E-04	<1.00E-01	rt	B435	0 0 0 0 0	

4343. C₂₃H₂₇NO₈

Narceine

o-Veratric acid, 6-[[6-[2-(dimethylamino)ethyl]-2-methoxy-3,4-(methylenedioxy)phenyl]acetyl]-NIH 10760

RN: 131-28-2 **MP (°C):** 138**MW:** 445.47 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-03	5.791E-01	15	K059	2 2 2 0 1	
2.915E-03	1.299E+00	c	D004	0 0 0 0 0	
1.016E-02	4.525E+00	h	D004	0 0 0 0 0	

4344. C₂₃H₂₇N₃O₇

Minocycline

Dynacin

Minocin

RN: 10118-90-8 **MP (°C):****MW:** 457.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.137E-01	5.200E+01	25	B191	1 0 0 0 1	neutral pH

4345. C₂₃H₂₈ClN₃O₂S

Thiopropazate

1-(2-Acetoxyethyl)-4-[3-(2-chloro-10-phenothiazinyl)propyl]piperazine

RN: 84-06-0 **MP (°C):****MW:** 446.02 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	8.920E-03	24	G022	2 0 1 1 1	

4346. C₂₃H₂₈ClN₃O₅S

Glyburide

HB 419

Glibenclamide

Diabeta

1-((*p*-(2-(5-Chloro-*o*-anisamido)ethyl)phenyl)-sulfonyl)-3-cyclohexylurea**RN:** 10238-21-8 **MP (°C):** 169**MW:** 494.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.137E-05	5.615E-03	22	M382	2 1 1 1 1	average of 2
6.275E-05	3.100E-02	25	G088	1 1 1 1 0	
1.000E-05	4.940E-03	25	Z410	0 0 0 0 0	EFG
8.097E-06	4.000E-03	27	H093	1 0 1 1 0	
2.024E-05	1.000E-02	ns	K444	0 0 0 0 0	

4347. C₂₃H₂₈O₇

Prednisone acetate

Pregna-1,4-diene-3,11,20-trione, 21-(acetyloxy)-17-hydroxy-

RN: 125-10-0 **MP (°C):****MW:** 416.48 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.522E-05	2.300E-02	25	K003	2 1 1 1 1	

4348. C₂₃H₂₉ClFN₃O₄

Cisapride

4-Amino-5-chloro-*N*-[1-[3-(4-fluorophenoxy)propyl]-3-methoxy-4-piperidyl]-2-methoxybenzamide**RN:** 81098-60-4 **MP (°C):****MW:** 465.96 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	9.319E-03	30	A417	0 0 0 0 0	pH 8.2
4.000E-04	1.864E-01	30	A417	0 0 0 0 0	pH 3.6

4349. C₂₃H₃₁Cl₂NO₃

Estramustine

Estradiol 3-[bis(2-chloroethyl)carbamate]

3-[bis(2-Chloroethyl)carbamate]

RN: 2998-57-4 **MP (°C):****MW:** 440.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~2.27E-06	~1.00E-03	30	L334	1 0 1 1 0	

4350. C₂₃H₃₁FO₆

9α-Fluorohydrocortisone acetate

Pregn-4-ene-3,20-dione, 21-(acetyloxy)-9-fluoro-11,17-dihydroxy-, (11β)-

RN: 514-36-3 MP (°C):

MW: 422.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.278E-04	5.400E-02	25	K021	1 2 2 2 1	

4351. C₂₃H₃₁N₅O₄

Benzoic acid, 3-[(dipropylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c]pyridin-1-yl)methoxy]ethyl ester

1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.

RN: 137605-71-1 MP (°C):

MW: 441.53 BP (°C): 674.6

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.944E-04	1.300E-01	21	B419	1 1 2 2 1	int

4352. C₂₃H₃₁O₇

Cortisone-21-hemi-succinate

RN: MP (°C):

MW: 419.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.768E-04	2.000E-01	ns	E307	0 0 0 0 0	

4353. C₂₃H₃₂O₂

Medrogestone

Pregna-4,6-diene-3,20-dione, 6,17-dimethyl-

RN: 977-79-7 MP (°C): 144

MW: 340.51 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.345E-06	1.820E-03	25	L033	1 0 2 1 2	

4354. C₂₃H₃₂O₄

Deoxycorticosterone acetate

Pregn-4-ene-3,20-dione, 21-(acetyloxy)-

RN: 56-47-3 MP (°C): 156

MW: 372.51 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.074E-05	4.000E-03	25	K003	2 1 1 1 1	

4355. C₂₃H₃₂O₆

Hydrocortisone acetate

Hydrocortisone-21-acetate

Cortisol acetate

Cortisol 21-acetate

RN: 50-03-3**MP (°C):** 223dec**MW:** 404.51**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.486E-05	1.410E-02	25	C037	2 1 2 2 2	
1.555E-05	6.290E-03	25	H098	1 0 2 0 2	
1.555E-05	6.290E-03	25	H320	0 0 0 0 0	
1.550E-05	6.270E-03	25	H320	0 0 0 0 0	
2.472E-05	1.000E-02	25	K003	2 1 1 1 1	
3.461E-05	1.400E-02	25	K021	1 2 2 2 1	
2.472E-05	1.000E-02	25	M023	1 0 2 1 0	
2.472E-05	1.000E-02	ns	M169	0 0 0 0 1	
1.904E-05	7.700E-03	ns	N323	0 0 0 0 0	

4356. C₂₃H₃₄O₃

Testosterone butyrate

Androst-4-en-3-one, 17-(1-oxobutoxy)-, (17bet)-

RN: 3410-54-6 **MP (°C):****MW:** 358.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.406E-06	5.039E-04	25	J004	1 0 1 1 2	
1.403E-06	5.030E-04	ns	B057	0 2 1 1 2	

4357. C₂₃H₃₄O₃

5,6-Dehydroisoandrosterone butyrate

Androst-5-en-17-one, 3-(1-oxobutoxy)-, (3β)-

RN: 15253-51-7 **MP (°C):****MW:** 358.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.231E+00	4.413E+02	ns	B057	0 2 1 1 2	

4358. C₂₃H₃₄O₃17- α -Methyltestosterone propionate**RN:** **MP (°C):****MW:** 358.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.845E-06	1.020E-03	ns	B057	0 2 1 1 2	

4359. C₂₃H₃₄O₄

Digitoxigenin

Card-20(22)-enolide, 3,14-dihydroxy-, (3 β ,5 β)-

RN: 143-62-4 MP (°C):

MW: 374.53 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	1.124E-02	30	O321	0 0 0 0 0	

4360. C₂₃H₃₅NOS

5-Pregnene-20-one-3-spiro-2'-(1',2'-thiazolidine)

RN: MP (°C): 127-136

MW: 373.61 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~1.34E-05	~5.00E-03	ns	B199	0 0 0 0 0	

4361. C₂₃H₃₆N₂O₂

Finasteride

Proscar

RN: 98319-26-7 MP (°C):

MW: 372.56 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.074E-04	4.000E-02	amb	L434	0 0 0 0 0	

4362. C₂₃H₃₆O₃

Androstanolone butyrate

Androstan-3-one, 17-(1-oxobutoxy)-, (5 α ,17 β)-

RN: 18069-66-4 MP (°C):

MW: 360.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.220E-06	4.400E-04	ns	B057	0 2 1 1 2	

4363. C₂₃H₃₈O₃Hexadecyl *p*-hydroxybenzoate

Hexadecyl 4-hydroxybenzoate

RN: 71067-09-9 MP (°C):

MW: 362.56 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.045E-03	3.789E-01	25	D081	1 2 2 1 2	

4364. C₂₃H₄₀O₅

4-Nonylphenol tetraethoxylate
p-Nonylphenol tetraethoxylate

RN: 7311-27-5 **MP (°C):**
MW: 396.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.929E-05	7.650E-03	20.5	A335	0 0 0 0 0	
1.930E-05	7.654E-03	20.5	A335	0 0 0 0 0	

4365. C₂₄H₁₂

Coronene
Coronen

RN: 191-07-1 **MP (°C):** 438
MW: 300.36 **BP (°C):** 525

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.680E-09	1.406E-06	20	E009	1 0 0 1 2	
3.329E-10	1.000E-07	25	B319	2 0 1 2 1	
4.661E-10	1.400E-07	25	M064	1 1 2 2 1	
4.660E-10	1.400E-07	25	M342	1 0 1 1 2	

4366. C₂₄H₂₀N₂

N,N'-Diphenylbenzidine

RN: 531-91-9 **MP (°C):** 247
MW: 336.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.783E-07	6.000E-05	50	K068	1 0 2 2 0	buffer
1.783E-07	6.000E-05	rt	K068	0 0 2 2 0	buffer

4367. C₂₄H₂₂N₂O₂

G-3

p-Phenylpropylphenylbutazone
3,5-Pyrazolidinedione, 1,2-diphenyl-4-(3-phenylpropyl)-

RN: 32060-78-9 **MP (°C):**
MW: 370.46 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.779E-04	1.400E-01	ns	B158	0 0 0 0 1	pH 7.0

4368. C₂₄H₂₆N₂O₄

Carvedilol

RN: 72956-09-3

MP (°C):

MW: 406.49

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	4.492E-04	22.5	B440	0 0 0 0 0	
7.380E-05	3.000E-02	ns	S469	0 0 0 0 0	

4369. C₂₄H₂₆N₄O₂

Methyldiantipyrylmethane

MDAM

RN: 1606-56-0

MP (°C):

MW: 402.50

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.118E-03	4.498E-01	20	P054	0 0 0 0 0	

4370. C₂₄H₂₆N₄S₂

Methyldithiopyrylmethane

3H-Pyrazole-3-thione, 4,4'-ethylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-

RN: 74713-70-5 MP (°C): 229

MW: 434.63 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-04	2.173E-01	ns	D087	0 2 0 0 1	

4371. C₂₄H₂₇BrN₆O₁₀

C.I. Disperse blue 79

2'-Acetylamino-4'-(bis(acetoxyethyl)amino)-6-bromo-2,4-dinitro-5'-ethoxyazobenzene

RN: 12239-34-8 MP (°C): 146

MW: 639.43 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-09	6.394E-07	25	B333	0 0 0 0 0	

4372. C₂₄H₂₇N

Prenylamine

N-(3,3-Diphenylpropyl)- α -methylphenylethylamine

RN: 390-64-7 MP (°C): 36.5

MW: 329.49 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.517E-04	5.000E-02	37	C054	2 0 2 1 0	

4373. C₂₄H₂₉N₅O₃

Valsartan

(2S)-3-Methyl-2-[pentanoyl-[[4-[2-(2H-tetrazol-5-yl)phenyl]phenyl]methyl]amino]butanoic acid

RN: 137862-53-4 **MP (°C):****MW:** 435.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.951E-04	8.499E-02	25	C431	0 0 0 0 0	

4374. C₂₄H₃₀F₂O₆

Fluocinolone acetonide

6α,9α-Difluoro-16α hydroxyprednisolone-16,17-acetonide

6α,9α-Difluoro-16α,17α-isopropylidenedioxy-1,4-pregnadiene-3,20-dione

RN: 67-73-2 **MP (°C):** 260.5**MW:** 452.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.387E-04	1.080E-01	25	K021	1 2 2 2 1	
4.641E-05	2.100E-02	25	O001	2 0 2 2 2	
2.210E-04	1.000E-01	25	P008	0 0 0 0 0	EFG

4375. C₂₄H₃₁ClO₇

Loteprednol etabonate

Lenoxin

Androsta-1,4-diene-17-carboxylic acid

17-[(Ethoxycarbonyl)oxy]-11-hydroxy-3-oxo-chloromethyl ester, (11b,17a)-

RN: 82034-46-6 **MP (°C):****MW:** 466.96 **BP (°C):** 600.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.14E-06	<1.00E-03	23	B409	1 0 0 0 1	

4376. C₂₄H₃₁FO₅S

Timobesone acetate

17-β-Methythiocarbonyl-9α-fluoro-11β

RN: 79578-14-6 **MP (°C):****MW:** 450.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-03	2.703E+00	25	O318	0 0 0 0 0	

4377. C₂₄H₃₁FO₆

Triamcinolone acetonide

9α-Fluoro-16α-hydroxyprednisolone acetonide

Triamcinolone 16α,17-acetonide

Aristoderm

Adcortyl-A

RN: 76-25-5**MP (°C):** 293**MW:** 434.51**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.205E-05	4.000E-02	23	F025	1 0 0 0 0	
9.436E-05	4.100E-02	25	K021	1 2 2 2 1	
6.076E-04	2.640E-01	25	L009	1 0 0 1 1	
4.833E-05	2.100E-02	28	B055	2 0 2 2 2	
4.027E-05	1.750E-02	28	B056	1 2 1 1 2	
5.869E-05	2.550E-02	37	B055	2 0 2 2 2	
4.764E-05	2.070E-02	37	B056	1 2 1 1 2	
9.205E-05	4.000E-02	37	F025	1 0 0 0 0	
7.733E-05	3.360E-02	50	B055	2 0 2 2 2	
6.099E-05	2.650E-02	50	B056	1 2 1 1 2	
2.532E-04	1.100E-01	amb	L434	0 0 0 0 0	

4378. C₂₄H₃₁FO₆

Betamethasone acetate

Betamethasone-17-acetate

9α-Fluoro-16β-methylprednisolone-21-acetate

RN: 987-24-6 **MP (°C):** 200dec**MW:** 434.51 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.904E-05	3.000E-02	25	K003	2 1 1 1 1	

4379. C₂₄H₃₁FO₆

Dexamethasone acetate

Dexamethasone-17-acetate

Dexamethasone acetate

RN: 1177-87-3 **MP (°C):** 263**MW:** 434.51 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.992E-05	1.300E-02	25	K003	2 1 1 1 1	
6.214E-05	2.700E-02	37	D026	0 0 0 0 0	

4380. C₂₄H₃₁NO₄

Drotaverine

1-(3,4-Diethoxybenzylidene)-6,7-diethoxy-1,2,3,4-tetrahydroisoquinoline

RN: 14009-24-6 MP (°C):

MW: 397.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.459E-02	1.375E+01	37	C054	2 0 2 1 2	

4381. C₂₄H₃₂N₂O₉

Enalapril maleate

L-Proline, 1-[N-[1-(ethoxycarbonyl)-3-phenylpropyl]-L-alanyl]-,

(S)-1-(N-(1-(Ethoxycarbonyl)-3-phenylpropyl)-L-alanyl)-L-proline, (Z)-2-butenedioate salt

RN: 76095-16-4 MP (°C):

MW: 492.53 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.264E-02	2.100E+01	25	A412	1 0 2 2 1	int

4382. C₂₄H₃₂O₄

Ethynodiol diacetate

Ovulen-50

RN: 297-76-7 MP (°C): 126

MW: 384.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.641E-06	1.400E-03	25	L027	1 0 0 0 2	

4383. C₂₄H₃₂O₄S

Spironolactone

17-Hydroxy-7 α -mercapto-3-oxo-17 α -pregn-4-ene-21-carboxylic acid γ -lactone acetate

Spiractin

RN: 52-01-7 MP (°C): 134

MW: 416.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.200E-06	2.999E-03	25	A348	0 0 0 0 0	
5.281E-05	2.200E-02	25	C037	2 1 2 2 2	
5.281E-05	2.200E-02	25	G084	2 0 2 2 1	
4.801E-05	2.000E-02	25	G095	2 1 2 2 1	
6.649E-05	2.770E-02	37	K092	2 0 0 1 2	
2.400E-05	1.000E-02	ns	K444	0 0 0 0 0	

4384. C₂₄H₃₂O₅

7-Carboxylic acid methyl ester canrenone

RN: **MP (°C):**
MW: 400.52 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.960E-04	7.850E-02	37	C004	0 0 0 0 0	EFG

4385. C₂₄H₃₂O₆

Cortisone 17-propionate

Pregn-4-ene-3,11,20-trione, 21-hydroxy-17-(1-oxopropoxy)-

RN: 136370-32-6 **MP (°C):**
MW: 416.52 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.921E-05	8.000E-03	25	M023	1 0 2 1 0	

4386. C₂₄H₃₃FO₆

Flurandrenolone

Fludroxicortide

6-Fluoro-16α-hydroxyhydrocortisone-16,17-acetonide

RN: 1524-88-5 **MP (°C):**
MW: 436.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.758E-04	2.950E-01	25	K021	1 2 2 2 1	

4387. C₂₄H₃₄N₂O

Bepridil

1-Isobutoxy-2-pyrrolidino-3-N-benzylanilino-propane

Bepadin

RN: 64706-54-3 **MP (°C):**
MW: 366.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.027E-02	7.430E+00	37	N032	1 0 1 1 2	

4388. C₂₄H₃₄N₂O₃

Lysine estrone ester

RN: **MP (°C):**
MW: 398.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-01	1.260E+02	ns	A074	0 0 0 0 0	EFG

4389. C₂₄H₃₄O₅

Dehydrocholic acid

3,7,12-Trioxo-5β-cholanic acid

RN: 81-23-2 **MP (°C):** 237
MW: 402.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.472E-04	1.800E-01	15	G081	1 0 1 1 1	
1.615E-04	6.500E-02	30	O321	0 0 0 0 0	
1.600E-04	6.441E-02	30	O321	0 0 0 0 0	

4390. C₂₄H₃₄O₆

Hydrocortisone propionate

Hydrocortisone-21-propionate

RN: 6677-98-1 **MP (°C):**
MW: 418.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.772E-05	1.160E-02	25	H098	1 0 2 0 2	
2.772E-05	1.160E-02	25	H320	0 0 0 0 0	
2.770E-05	1.159E-02	25	H320	0 0 0 0 0	

4391. C₂₄H₃₆O₃

Testosterone valerate

Androst-4-en-3-one, 17-[(1-oxopentyl)oxy]-, (17β)-

Testosterone 17-valerate

RN: 3129-43-9 **MP (°C):**
MW: 372.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.778E-07	2.898E-04	25	J004	1 0 1 1 2	
7.811E-07	2.910E-04	ns	B057	0 2 1 1 2	

4392. C₂₄H₃₆O₃

5,6-Dehydroisoandrosterone valerate

Androst-5-en-17-one, 3-[(1-oxopentyl)oxy]-, (3β)-

RN: 7642-68-4 **MP (°C):**
MW: 372.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.061E-05	7.680E-03	ns	B057	0 2 1 1 2	

4393. C₂₄H₃₈O₃

Androstanolone valerate

Androstan-3-one, 17-[(1-oxopentyl)oxy]-, (5 α ,17 β)-

RN: 26271-72-7 MP (°C):

MW: 374.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.143E-07	3.050E-04	ns	B057	0 2 1 1 2	

4394. C₂₄H₃₈O₄

Di-2-ethylhexyl isophthalate

D-(2-Ethylhexyl) isophthalate

Dioctyl isophthalate

RN: 137-89-3 MP (°C):

MW: 390.57 BP (°C): 400

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.816E-08	1.100E-05	24	H116	2 1 0 0 2	

4395. C₂₄H₃₈O₄

Octyl phthalate

Di(2-ethylhexyl)phthalate

Di-(2-ethylhexyl)-phthalate

Di-*sec*-octyl phthalate

bis(2-Ethylhexyl) phthalate

bis-(2-Ethylhexyl) 1,2-benzenedicarboxylate

RN: 117-81-7 MP (°C): -50

MW: 390.57 BP (°C): 386.9

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.560E-04	9.999E-02	20	F070	1 0 0 0 1	<i>sic</i>
1.050E-07	4.101E-05	20	L300	2 1 0 2 2	
1.536E-06	6.000E-04	22.5	G301	0 0 0 0 0	
7.297E-07	2.850E-04	24	H116	2 1 0 0 2	
6.913E-07	2.700E-04	25	D336	0 0 0 0 0	
1.280E-06	5.000E-04	25	F067	1 0 2 2 0	

4396. C₂₄H₃₈O₄

Apocholic acid

RN: 641-81-6 MP (°C): 175.5

MW: 390.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.048E-03	8.000E-01	15	G081	1 0 1 1 0	

4397. C₂₄H₃₈O₄

bis(Tereoctyl) phthalate

RN: MP (°C):

MW: 390.57 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.633E-08	2.200E-05	25	D336	0 0 0 0 0	

4398. C₂₄H₃₈O₄

bis(Isooctyl) phthalate

Diisooctyl phthalate

1,2-Benzenedicarboxylic acid diisooctyl ester

RN: 27554-26-3 MP (°C): -4

MW: 390.57 BP (°C): 239

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.024E-07	4.000E-05	25	D336	0 0 0 0 0	

4399. C₂₄H₃₈O₄bis(*n*-Octyl) phthalateDi-*n*-octyl phthalate

1,2-Benzenedicarboxylic acid

RN: 117-84-0 MP (°C): -25

MW: 390.57 BP (°C): 220

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.121E-08	2.000E-05	25	D336	0 0 0 0 0	

4400. C₂₄H₃₉NO₃

Acetaminophen palmitate

Acetaminophen hexadecanoate

RN: 54942-40-4 MP (°C): 117

MW: 389.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.283E-05	5.000E-03	25	B010	1 1 1 1 0	

4401. C₂₄H₄₀N₈O₄

Dipyridamole

2,6-bis(Diethanolamino)-4,8-dipiperidinopyrimido-[5,4-d]pyrimidin

Dipridacot

Dipyridamole

Persantin

Dipyridamol

RN: 58-32-2**MP (°C):****MW:** 504.64**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.649E-06	8.320E-04	22.5	B440	0 0 0 0 0	
7.000E-05	3.532E-02	30	A417	0 0 0 0 0	pH 5.2
3.200E-03	1.615E+00	30	A417	0 0 0 0 0	pH 3.7

4402. C₂₄H₄₀O₃

3β-Hydroxy-5β-cholanoic acid

7α-Hydroxy-5β-cholanoic acid

RN: MP (°C):**MW:** 376.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-07	6.779E-05	10	F307	1 2 2 2 2	pH 3.0
4.400E-07	1.657E-04	10	F307	1 2 2 2 2	pH 3.0
5.200E-07	1.958E-04	15	F307	1 2 2 2 2	pH 3.0
2.200E-07	8.285E-05	15	F307	1 2 2 2 2	pH 3.0
2.400E-07	9.038E-05	20	F307	1 2 2 2 2	pH 3.0
6.500E-07	2.448E-04	20	F307	1 2 2 2 2	pH 3.0
2.800E-07	1.054E-04	25	F307	1 2 2 2 2	pH 3.0
7.900E-07	2.975E-04	25	F307	1 2 2 2 2	pH 3.0
3.500E-07	1.318E-04	30	F307	1 2 2 2 2	pH 3.0
9.700E-07	3.653E-04	30	F307	1 2 2 2 2	pH 3.0
5.300E-07	1.996E-04	35	F307	1 2 2 2 2	pH 3.0
1.190E-06	4.481E-04	35	F307	1 2 2 2 2	pH 3.0
8.200E-07	3.088E-04	40	F307	1 2 2 2 2	pH 3.0
1.490E-06	5.611E-04	40	F307	1 2 2 2 2	pH 3.0
1.770E-06	6.666E-04	45	F307	1 2 2 2 2	pH 3.0
1.280E-06	4.820E-04	45	F307	1 2 2 2 2	pH 3.0
1.500E-06	5.649E-04	50	F307	1 2 2 2 2	pH 3.0
2.150E-06	8.097E-04	50	F307	1 2 2 2 2	pH 3.0

4403. C₂₄H₄₀O₃

Lithocholic acid

3 α -Hydroxy-5 β -cholan-24-oic acid3 α -Hydroxycholanic acid**RN:** 434-13-9 **MP (°C):** 184**MW:** 376.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.800E-08	1.431E-05	10	F307	1 2 2 2 2	pH 3.0
4.000E-08	1.506E-05	15	F307	1 2 2 2 2	pH 3.0
4.600E-08	1.732E-05	20	F307	1 2 2 2 2	pH 3.0
1.000E-06	3.766E-04	20	I012	1 2 2 1 0	pH 2.4
5.000E-08	1.883E-05	25	F307	1 2 2 2 2	pH 3.0
6.000E-08	2.260E-05	30	F307	1 2 2 2 2	pH 3.0
7.500E-08	2.824E-05	35	F307	1 2 2 2 2	pH 3.0
1.000E-06	3.766E-04	37	I012	1 2 2 1 0	pH 2.4
1.000E-07	3.766E-05	40	F307	1 2 2 2 2	pH 3.0
1.100E-07	4.142E-05	45	F307	1 2 2 2 2	pH 3.0
1.400E-07	5.272E-05	50	F307	1 2 2 2 2	pH 3.0

4404. C₂₄H₄₀O₄

Hyodeoxycholic acid

3 α ,6 β -Dihydroxy-5 α -cholanoic acid**RN:** 83-49-8 **MP (°C):** 198**MW:** 392.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.000E-05	3.926E-03	10	F307	1 2 2 2 2	pH 3.0
1.200E-05	4.711E-03	15	F307	1 2 2 2 2	pH 3.0
1.300E-05	5.104E-03	20	F307	1 2 2 2 2	pH 3.0
1.500E-05	5.889E-03	25	F307	1 2 2 2 2	pH 3.0
1.700E-05	6.674E-03	30	F307	1 2 2 2 2	pH 3.0
1.800E-05	7.067E-03	35	F307	1 2 2 2 2	pH 3.0
2.000E-05	7.852E-03	40	F307	1 2 2 2 2	pH 3.0
2.200E-05	8.637E-03	45	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	50	F307	1 2 2 2 2	pH 3.0

4405. C₂₄H₄₀O₄

Deoxycholic acid

Cholan-24-oic acid, 3,12-dihydroxy-, (3 α ,5 β ,12 α)-3 α ,12 α -Dihydroxy-5 β -cholanoic acid**RN:** 83-44-3 **MP (°C):** 176**MW:** 392.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-05	9.422E-03	10	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	15	F307	1 2 2 2 2	pH 3.0
6.113E-04	2.400E-01	15	G081	1 0 1 1 1	

(continued)

4405. C₂₄H₄₀O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.093E-04	2.000E-01	20	D041	1 0 0 0 0	
2.700E-05	1.060E-02	20	F307	1 2 2 2 2	pH 3.0
1.110E-04	4.358E-02	20	I012	1 2 2 1 2	pH 2.4
2.800E-05	1.099E-02	25	F307	1 2 2 2 2	pH 3.0
2.800E-05	1.099E-02	30	F307	1 2 2 2 2	pH 3.0
2.900E-05	1.138E-02	35	F307	1 2 2 2 2	pH 3.0
1.140E-04	4.475E-02	37	I012	1 2 2 1 2	pH 2.4
2.900E-05	1.138E-02	40	F307	1 2 2 2 2	pH 3.0
3.000E-05	1.178E-02	45	F307	1 2 2 2 2	pH 3.0
3.200E-05	1.256E-02	50	F307	1 2 2 2 2	pH 3.0

4406. C₂₄H₄₀O₄

Chenodeoxycholic acid

CDCA

RN: 474-25-9 MP (°C): 119
 MW: 392.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-05	9.815E-03	10	F307	1 2 2 2 2	pH 3.0
2.500E-05	9.815E-03	15	F307	1 2 2 2 2	pH 3.0
2.600E-05	1.021E-02	20	F307	1 2 2 2 2	pH 3.0
2.290E-04	8.990E-02	20	I012	1 2 2 1 2	pH 2.4
2.700E-05	1.060E-02	25	F307	1 2 2 2 2	pH 3.0
2.800E-05	1.099E-02	30	F307	1 2 2 2 2	pH 3.0
3.000E-05	1.178E-02	35	F307	1 2 2 2 2	pH 3.0
2.560E-04	1.005E-01	37	I008	1 0 0 1 2	
2.560E-04	1.005E-01	37	I012	1 2 2 1 2	pH 2.4
3.150E-05	1.237E-02	40	F307	1 2 2 2 2	pH 3.0
3.400E-05	1.335E-02	45	F307	1 2 2 2 2	pH 3.0
3.600E-05	1.413E-02	50	F307	1 2 2 2 2	pH 3.0
2.291E-04	8.994E-02	ns	R427	0 0 0 0 0	

4407. C₂₄H₄₀O₄

Ursodeoxycholic acid

UDCA

RN: 128-13-2 MP (°C): 203
 MW: 392.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-06	2.748E-03	10	F307	1 2 2 2 2	pH 3.0
7.500E-06	2.944E-03	15	F307	1 2 2 2 2	pH 3.0
8.000E-06	3.141E-03	20	F307	1 2 2 2 2	pH 3.0
5.100E-05	2.002E-02	20	I012	1 2 2 1 1	pH 2.4
9.000E-06	3.533E-03	25	F307	1 2 2 2 2	pH 3.0
1.000E-05	3.926E-03	30	F307	1 2 2 2 2	pH 3.0 (continued)

4407. C₂₄H₄₀O₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.150E-05	4.515E-03	35	F307	1 2 2 2 2	pH 3.0
5.300E-05	2.081E-02	37	I008	1 0 0 1 1	
5.300E-05	2.081E-02	37	I012	1 2 2 1 1	pH 2.4
1.200E-05	4.711E-03	40	F307	1 2 2 2 2	pH 3.0
1.300E-05	5.104E-03	45	F307	1 2 2 2 2	pH 3.0
1.400E-05	5.496E-03	50	F307	1 2 2 2 2	pH 3.0
8.556E-04	3.359E-01	ns	K446	0 0 0 0 0	

4408. C₂₄H₄₀O₅3 α , 6 α , 7 α -Trihydroxy-5 β -cholanate

RN: MP (°C):
MW: 408.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.700E-05	1.512E-02	10	F307	1 2 2 2 2	pH 3.0
3.800E-05	1.553E-02	15	F307	1 2 2 2 2	pH 3.0
4.100E-05	1.675E-02	20	F307	1 2 2 2 2	pH 3.0
4.500E-05	1.839E-02	25	F307	1 2 2 2 2	pH 3.0
5.500E-05	2.247E-02	30	F307	1 2 2 2 2	pH 3.0
6.900E-05	2.819E-02	35	F307	1 2 2 2 2	pH 3.0
8.600E-05	3.514E-02	40	F307	1 2 2 2 2	pH 3.0
1.160E-04	4.740E-02	45	F307	1 2 2 2 2	pH 3.0
1.600E-04	6.537E-02	50	F307	1 2 2 2 2	pH 3.0

4409. C₂₄H₄₀O₅

Ursocholic acid

3 α ,7 β ,12 α -Trihydroxy-5 β -cholanoic acid

RN: 2955-27-3 MP (°C):
MW: 408.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.590E-03	6.496E-01	10	F307	1 2 2 2 2	pH 3.0
1.610E-03	6.578E-01	15	F307	1 2 2 2 2	pH 3.0
1.640E-03	6.701E-01	20	F307	1 2 2 2 2	pH 3.0
1.670E-03	6.823E-01	25	F307	1 2 2 2 2	pH 3.0
1.710E-03	6.987E-01	30	F307	1 2 2 2 2	pH 3.0
1.762E-03	7.199E-01	35	F307	1 2 2 2 2	pH 3.0
1.828E-03	7.469E-01	40	F307	1 2 2 2 2	pH 3.0
1.872E-03	7.649E-01	45	F307	1 2 2 2 2	pH 3.0
2.000E-03	8.172E-01	50	F307	1 2 2 2 2	pH 3.0

4410. C₂₄H₄₀O₅

Cholic acid

Cholsaeure

RN: 81-25-4

MP (°C): 198

MW: 408.58

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.210E-04	9.030E-02	10	F307	1 2 2 2 2	pH 3.0
6.486E-04	2.650E-01	15	F300	1 0 0 0 0	
2.140E-04	8.744E-02	15	F307	1 2 2 2 2	pH 3.0
6.853E-04	2.800E-01	15	G081	1 0 1 1 1	
6.851E-04	2.799E-01	20	D041	1 0 0 0 1	
2.247E-04	9.180E-02	20	E008	1 0 2 0 2	average of 3
2.200E-04	8.989E-02	20	F307	1 2 2 2 2	pH 3.0
4.280E-04	1.749E-01	20	I012	1 2 2 1 2	pH 2.4
2.350E-04	9.602E-02	25	F307	1 2 2 2 2	pH 3.0
2.670E-04	1.091E-01	30	F307	1 2 2 2 2	pH 3.0
3.240E-04	1.324E-01	35	F307	1 2 2 2 2	pH 3.0
4.600E-04	1.879E-01	37	I012	1 2 2 1 2	pH 2.4
3.830E-04	1.565E-01	40	F307	1 2 2 2 2	pH 3.0
4.830E-04	1.973E-01	45	F307	1 2 2 2 2	pH 3.0
6.390E-04	2.611E-01	50	F307	1 2 2 2 2	pH 3.0

4411. C₂₄H₅₀

Tetracosane

n-Tetracosane

Alkane C(24)

RN: 646-31-1

MP (°C): 54

MW: 338.67

BP (°C): 391.3

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.264E-02	4.282E+00	321	S355	1 1 1 2 0	EFG
8.878E-02	3.007E+01	369	S355	1 1 1 2 0	EFG

4412. C₂₄H₅₁OPtri-*n*-Octylphosphine oxide

TOPO

Trioctylphosphine oxide

RN: 78-50-2

MP (°C):

MW: 386.65

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.242E-06	2.800E-03	0	O002	2 0 2 2 1	
3.880E-06	1.500E-03	25	O002	2 0 2 2 1	

4413. C₂₄H₅₁O₃P

Dibutyl hexadecyl phosphonate

Phosphonic acid, hexadecyl-, dibutyl ester

RN: 84869-93-2 MP (°C):

MW: 418.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<4.78E-04	<2.00E-01	25	B070	1 2 0 1 0	

4414. C₂₄H₅₁O₄P*tris*-(2-Ethylhexyl) phosphate

Disflamoll TOF

TEHP

Flexol TOF

RN: 78-42-2 MP (°C):

MW: 434.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.380E-06	6.000E-04	24	H116	2 1 0 0 2	

4415. C₂₄H₅₄OSn₂

bis(Tributyltin) oxide

6-Oxa-5,7-distannaundecane, 5,5,7,7-tetrabutyl-

RN: 56-35-9 MP (°C):

MW: 596.08 BP (°C): 180

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.678E-04	1.000E-01	rt	M161	0 0 0 0 2	

4416. C₂₅H₂₂O₁₀

Silybin

Silibinin

Silybum substance E6

Silymarin I

RN: 22888-70-6 MP (°C):

MW: 482.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.788E-05	4.240E-02	19.99	B439	0 0 0 0 0	
1.119E-04	5.400E-02	24.99	B439	0 0 0 0 0	
1.432E-04	6.910E-02	29.99	B439	0 0 0 0 0	
1.726E-04	8.329E-02	34.99	B439	0 0 0 0 0	
2.066E-04	9.969E-02	39.99	B439	0 0 0 0 0	

4417. C₂₅H₂₄F₆N₄

Hydramethylnon

Amdro

Comat

Amidinohydrazone;

Wipeout

Tetrahydro-5,5-dimethyl-2(1H)-pyrimidinone[3-[4-(trifluoromethyl)phenyl]-1-[2-[4-(trifluoromethyl)phenyl]ethenyl]-2-propenylidene]hydrazone

RN: 67485-29-4 **MP (°C):** 185-190**MW:** 494.49 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.202E-08	5.945E-06	ns	R427	0 0 0 0 0	

4418. C₂₅H₂₄N₂O₂S

G-8

o,p-Dimethylphenylthioethylphenylbutazone

3,5-Pyrazolidinedione, 1,2-diphenyl-4-[2-(2,4-xylylthio)ethyl]-

RN: 102892-46-6 **MP (°C):****MW:** 416.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.121E-04	1.300E-01	ns	B158	0 0 0 0 1	pH 7.0

4419. C₂₅H₂₈N₄O₂

Ethyldantipyrylmethane

EDAM

RN: 61358-28-9 **MP (°C):****MW:** 416.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.601E-04	1.500E-01	20	P054	0 0 0 0 0	

4420. C₂₅H₂₈O₃

Estradiol benzoate

Estradiol monobenzoate

7 β -Estradiol-3-benzoate**RN:** 50-50-0 **MP (°C):** 190**MW:** 376.50 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.062E-06	4.000E-04	25	K003	2 1 1 1 1	
1.072E-06	4.034E-04	ns	R427	0 0 0 0 0	

4421. C₂₅H₂₈O₃

Ethofenprox

1-((2-(4-Ethoxyphenyl)-2-methylpropoxy)methyl)-3-phenoxybenzene

Etofenprox

Zoecon

MTI-500

Trebon

RN: 80844-07-1 MP (°C):

MW: 376.50 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.512E-09	9.457E-07	ns	R427	0 0 0 0 0	

4422. C₂₅H₂₉I₂NO₃

Amiodarone

Cordarone

Aratac

RN: 1951-25-3 MP (°C):

MW: 645.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<6.72E-08	<4.34E-05	22.5	B440	0 0 0 0 0	
1.110E-03	7.164E-01	25	B337	2 2 2 1 2	

4423. C₂₅H₃₁FO₈

Triamcinolone 16, 21-diacetate

Pregna-1,4-diene-3,20-dione, 16,21-bis(acetyloxy)-9-fluoro-11,17-dihydroxy-, (11β,16alpha)-

RN: 67-78-7 MP (°C): 235

MW: 478.52 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.003E-04	4.800E-02	25	F026	0 0 0 0 0	

4424. C₂₅H₃₁NO₂

3-Hydroxy-17β-{[(1-methyl-1,4-dihydropyridin-3-yl)-carbonyl]oxy}-estra-1,3,5(10)-triene

RN: MP (°C):

MW: 377.53 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.743E-07	6.580E-05	25	B366	0 0 0 0 0	

4425. C₂₅H₃₄O₃

Norethindrone dimethylpropionate

19-Norpregn-4-en-20-yn-3-one, 17-(2,2-dimethyl-1-oxopropoxy)-, (17 α)-

RN: 65445-09-2 MP (°C):

MW: 382.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.894E-08	3.020E-05	25	L078	1 0 1 2 2	

4426. C₂₅H₃₄O₆

Budesonide

16,17-Butylidenebis(oxy)-11-,21-dihydroxypregna-1,4-diene-3,20-dione

Rhinocort

RN: 51333-22-3 MP (°C):

MW: 430.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-05	2.153E-02	ns	F327	0 0 1 2 2	

4427. C₂₅H₃₄O₉

6-(1,3-Dihydro-7-acetate-5-methoxy-4-methyl-1-oxoisobenzofuran-6-yl)-4-methyl-4-hexanoic solketal ester

RN: MP (°C):

MW: 478.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.881E-05	9.000E-03	25	L333	1 1 1 1 0	

4428. C₂₅H₃₅N₅O₄

Benzoic acid, 3-[(dibutylamino)methyl]-, 2-[(6-amino-4,5-dihydro-4-oxo-1H-imidazo[4,5-c]pyridin-1-yl)methoxy]ethyl ester

1H-Imidazo[4,5-c]pyridine, benzoic acid deriv.

RN: 137605-73-3 MP (°C):

MW: 469.59 BP (°C): 688.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.278E-05	6.000E-03	21	B419	1 1 2 2 1	int

4429. C₂₅H₃₆N₄O₇

Nonyloxycarbonyl-mitomycin C

2'-(2-Hexanoyl-2-pentanyl-acetyl)-6-methoxypurine arabinoside

RN: MP (°C):

MW: 504.59 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-07	1.261E-04	25	M316	1 1 1 1 2	
2.020E-03	1.019E+00	37	C348	0 0 0 0 0	pH 7.00

4430. C₂₅H₃₆O₆

Hydrocortisone butyrate

Hydrocortisone-21-butyrate

11,17-Dihydroxy-21-(1-oxobutoxy)-pregn-4-ene-3,20-dione

RN: 6677-99-2 MP (°C):

MW: 432.56 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.787E-05	7.730E-03	25	H098	1 0 2 0 2	
1.787E-05	7.730E-03	25	H320	0 0 0 0 0	
1.780E-05	7.700E-03	25	H320	0 0 0 0 0	

4431. C₂₅H₃₆O₇5,16-β-Dihydroxy-6-β-methyl-3,11-dioxo-5-α-pregn-17(20)-ene-*cis*-20-carboxylic acid methyl ester cycl

RN: MP (°C):

MW: 448.56 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.672E-04	7.500E-02	ns	K029	0 0 2 1 1	

4432. C₂₅H₄₀O₃Si₂

Norethindrone pentamethyldisiloxyl ether

RN: MP (°C):

MW: 444.77 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.301E-07	1.023E-04	25	L078	1 0 1 2 2	

4433. C₂₅H₄₂O₃Octadecyl-*p*-hydroxybenzoate

RN: 71067-10-2 **MP (°C):**
MW: 390.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.343E-04	3.259E-01	25	D081	1 2 2 1 2	

4434. C₂₅H₄₄

Nonadecylbenzene

1-Phenylnonadecane

RN: 29136-19-4 **MP (°C):**
MW: 344.63 **BP (°C):** 419

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.530E-02	5.272E+00	328	S355	1 1 1 2 0	EFG
2.396E-01	8.257E+01	363	S355	1 1 1 2 0	EFG

4435. C₂₅H₄₄O₆

4-Nonylphenol pentaethoxylate

RN: 20636-48-0 **MP (°C):**
MW: 440.63 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.151E-05	9.480E-03	20.5	A335	0 0 0 0 0	
2.150E-05	9.473E-03	20.5	A335	0 0 0 0 0	

4436. C₂₅H₄₈O₄

Diocetyl azelate

Di(2-ethylhexyl) azelate

RN: 103-24-2 **MP (°C):**
MW: 412.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.423E-07	1.000E-04	25	F067	1 0 2 2 0	

4437. C₂₅H₅₄O₂P₂

bis(Di-*n*-hexyl-phosphinyl)methane
HDPM

RN: 2785-33-3 **MP (°C):**
MW: 448.66 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.426E-04	6.400E-02	0	O002	2 0 2 2 0	EFG
8.849E-05	3.970E-02	25	O002	2 0 2 2 1	average of 2
6.241E-05	2.800E-02	35	O002	2 0 2 2 0	EFG
4.458E-05	2.000E-02	40	O002	2 0 2 2 0	EFG
3.377E-03	1.515E+00	45	O002	2 0 2 2 0	EFG

4438. C₂₆H₁₈N₂O₄

Samaron violet
Mowilith red 3B(IG)

RN: 6408-72-6 **MP (°C):**
MW: 422.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-06	1.267E-03	98.59	M180	0 0 2 2 0	EFG
4.000E-06	1.690E-03	109.98	M180	0 0 2 1 0	EFG
4.500E-06	1.901E-03	120.54	M180	0 0 2 2 0	EFG
6.000E-06	2.535E-03	133.34	M180	0 0 2 2 0	EFG
8.000E-06	3.380E-03	141.78	M180	0 0 2 2 0	EFG

4439. C₂₆H₂₀N₂O₈S₂

1,5-Anthraquinone disulfonic acid anilide

RN: **MP (°C):**
MW: 552.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.210E-03	3.984E+00	18	F047	1 2 1 1 1	

4440. C₂₆H₂₀N₂O₈S₂

1,8-Anthraquinone disulfonic acid anilide

RN: **MP (°C):**
MW: 552.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.209E-02	2.326E+01	18	F047	1 2 1 1 1	

4441. C₂₆H₂₈Cl₂N₄O₄

Ketoconazole

(±)-*cis*-1-Acetyl-4-(4-[(2-[2,4-dichlorophenyl]-2-[1H-imidazol-1-ylmethyl]-1,3-dioxolan-4-yl)-methoxy]phenyl)piperazine**RN:** 65277-42-1 **MP (°C):****MW:** 531.44 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.505E-04	8.000E-02	37	C323	0 0 0 0 0	
1.882E-05	1.000E-02	amb	L434	0 0 0 0 0	EFG

4442. C₂₆H₂₈N₂

Cinnarizine

Stugeron

RN: 298-57-7 **MP (°C):****MW:** 368.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.035E-03	7.500E-01	ns	B155	0 0 1 1 0	EFG, pH 3.0

4443. C₂₆H₂₈N₄O₂

Propyldantipyrylmethane

PDAM

RN: 1461-17-2 **MP (°C):****MW:** 428.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	6.000E-02	20	P054	0 0 0 0 0	

4444. C₂₆H₂₉NO

Tamoxifen

Genox

Kessar

Nolvadex

(Z)-2-[4-(1,2-Diphenyl-1-butenyl)phenoxy]-*N,N*-dimethylethanamine

Tamoxen

RN: 10540-29-1 **MP (°C):****MW:** 371.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.550E+00	2.805E+03	25	B443	0 0 0 0 0	
		amb	L434	0 0 0 0 0	extrapolated

4445. C₂₆H₃₀Cl₂F₃NO

Halofantrine

1-(1,3-Dichloro-6-trifluoromethyl-9-phenanthryl)-3-di(*n*-butyl)aminopropanol

RN: 69756-53-2 MP (°C):

MW: 500.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.179E-06	5.900E-04	37	A423	0 0 0 0 0	

4446. C₂₆H₃₀N₄O₂

Isopropylidantipyrrylmethane

IPDAM

RN: 15536-49-9 MP (°C):

MW: 430.55 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.644E-04	2.000E-01	20	P054	0 0 0 0 0	

4447. C₂₆H₃₀N₄S₂

Propyldithiopyrrylmethane

3H-Pyrazole-3-thione, 4,4'-butylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-

RN: 57094-83-4 MP (°C): 222

MW: 462.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.400E-04	1.110E-01	ns	D087	0 2 0 0 1	

4448. C₂₆H₃₁ClN₂O₈S

Amlodipine

Amlodipine besylate

Norvasc

(RS)-3-Ethyl-5-methyl-2-(2-aminoethoxymethyl)-4-(2-chlorophenyl)-1,4-dihydro-6-methyl-3,5-pyridinedicarboxylate benzenesulfonate

RN: 88150-42-9 MP (°C):

MW: 567.06 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.76E-05	<1.00E-02	rt	B435	0 0 0 0 0	

4449. C₂₆H₃₂F₂O₇

Diflorasone diacetate

U-34865

RN: 33564-31-7 **MP (°C):**
MW: 494.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.314E-05	6.500E-03	25	F003	0 0 0 0 0	
1.254E-05	6.200E-03	37	F003	0 0 0 0 0	
2.629E-05	1.300E-02	50	F003	0 0 0 0 0	

4450. C₂₆H₃₂F₂O₇

Fluocinolide

Fluocinonide

Fluocinolone acetonide acetate

RN: 356-12-7 **MP (°C):**
MW: 494.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.072E-06	5.300E-04	25	O001	2 0 2 2 2	
2.022E-05	1.000E-02	25	P008	0 0 0 0 0	EFG

4451. C₂₆H₃₂O₃

Testosterone benzoate

Androst-4-en-3-one, 17-(benzoyloxy)-, (17 β)-

RN: 2088-71-3 **MP (°C):**
MW: 392.54 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.312E-05	1.300E-02	25	L342	1 0 1 1 2	

4452. C₂₆H₃₆O₃

Norethisterone heptanoate

RN: **MP (°C):**
MW: 396.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.521E-07	6.030E-05	25	E301	1 0 1 1 2	

4453. C₂₆H₃₆O₆

Prednisolone 21-trimethylacetate

Prednisolone acetate

RN: 52-21-1**MP (°C):** 233**MW:** 444.57**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.609E-05	1.160E-02	25	C037	2 1 2 2 2	
6.298E-05	2.800E-02	25	K021	1 2 2 2 1	
2.699E-05	1.200E-02	ns	N302	0 2 1 2 1	

4454. C₂₆H₃₇FO₅

Dexamethasone TBA

RN: 448.58**MP (°C):**
BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.229E-05	1.000E-02	37	D026	0 0 0 0 0	

4455. C₂₆H₃₈NO₈

Glucosamine testosterone

17-β-(4-Androsten-3-one)-N-2-(2-desoxyglucosyl)

RN: 492.59**MP (°C):** 185–190
BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.332E-03	6.560E-01	25	L009	1 0 0 1 1	

4456. C₂₆H₃₈O₄

Trimethylcyclohexyl phthalate

bis(*cis*-3,3,5-Trimethylcyclohexyl) phthalate**RN:** 245652-81-7 **MP (°C):** 93
MW: 414.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.894E-07	1.200E-04	24	H116	2 1 0 0 2	

4457. C₂₆H₃₈O₆

Hydrocortisone valerate
Hydrocortisone-21-valerate

RN: 6678-00-8 **MP (°C):**
MW: 446.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.830E-06	3.050E-03	25	H098	1 0 2 0 2	
6.830E-06	3.050E-03	25	H320	0 0 0 0 0	
6.780E-06	3.028E-03	25	H320	0 0 0 0 0	

4458. C₂₆H₃₉NO₃S

4-Pregnene-20-one-3-spiro-2'-(4'-ethoxycarbonyl-1',3'-thiazolidine)

RN: **MP (°C):** 131–135
MW: 445.67 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
~3.81E-06	~1.70E-03	ns	B199	0 0 0 0 0	

4459. C₂₆H₄₃NO₃

Acetaminophen stearate
Acetaminophen octadecanoate
Stearoyl acetaminophen
Octadecanoic acid, 4-(acetylamino)phenyl ester
Acetanilide, 4'-hydroxy-, stearate (ester)

RN: 20675-22-3 **MP (°C):** 117
MW: 417.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.197E-05	5.000E-03	25	B010	1 1 1 1 0	
3.592E-05	1.500E-02	37	D029	0 0 0 0 0	

4460. C₂₆H₄₃NO₆

Glycocholic acid
Glycine, N-[(3 α ,5 β ,7 α ,12 α)-3,7,12-trihydroxy-24-oxocholan-24-yl]-

RN: 475-31-0 **MP (°C):** 130
MW: 465.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.085E-04	3.299E-01	20	E035	1 2 0 0 1	
2.188E-03	1.019E+00	60	E035	1 2 0 0 2	
5.035E-03	2.344E+00	80	E035	1 2 0 0 2	
1.810E-02	8.428E+00	100	E035	1 2 0 0 1	

4461. C₂₆H₅₀O₄

Diocetyl sebacate

Sebacic acid bis(2-ethylhexyl) ester

RN: 122-62-3 **MP (°C):** -67
MW: 426.69 **BP (°C):** 248

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.344E-07	1.000E-04	25	F067	1 0 2 2 0	

4462. C₂₆H₅₆O₂P₂bis(Di-*n*-hexyl-phosphinyl)ethane

HDPE

RN: 2785-34-4 **MP (°C):**
MW: 462.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-05	1.300E-02	0	O002	2 0 2 2 1	EFG
6.484E-06	3.000E-03	25	O002	2 0 2 2 1	
6.484E-06	3.000E-03	60	O002	2 0 2 2 1	EFG

4463. C₂₇H₂₂Cl₂N₄

Clofazimine

Lamprene

N,5-bis(4-Chlorophenyl)-3,4-dihydro-3-((1-methylethyl)imino)-2-phenazinamine
 3-(*p*-Chloroanilino)-10-(*p*-chlorophenyl)-2,10-dihydro-2-(isopropylimino)phenazine

RN: 2030-63-9 **MP (°C):** 211
MW: 473.41 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.11E-06	<1.00E-03	ns	B404	0 2 1 1 0	
2.112E-05	1.000E-02	ns	K444	0 0 0 0 0	
2.000E-04	9.468E-02	ns	O322	0 0 0 0 0	EFG

4464. C₂₇H₂₉NO₁₁

Adriamycin

Adriblastin

RN: 23214-92-8 **MP (°C):** 205
MW: 543.53 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.607E-02	1.961E+01	ns	I312	0 0 0 0 0	

4465. C₂₇H₃₀O₃

Norethindrone benzoate

RN: MP (°C):
MW: 402.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.019E-08	8.128E-06	25	L078	1 0 1 2 2	

4466. C₂₇H₃₂N₄O₂

Butyldiantipyrylmethane

BDAM

RN: 61358-30-3 MP (°C):
MW: 444.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.748E-05	3.000E-02	20	P054	0 0 0 0 0	

4467. C₂₇H₃₂N₄O₂

Isobutylidantipyrylmethane

IBDAM

RN: 16671-34-4 MP (°C):
MW: 444.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	6.000E-02	20	P054	0 0 0 0 0	

4468. C₂₇H₃₂N₄S₂

Isobutylidithiopyrylmethane

3H-Pyrazole-3-thione, 4,4'-(3-methylbutylidene)bis[1,2-dihydro-1,5-dimethyl-2-phenyl-

RN: 73429-89-7 MP (°C): 209
MW: 476.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-04	7.627E-02	ns	D087	0 2 0 0 1	

4469. C₂₇H₃₂O₁₄

Naringin

4H-1-Benzopyran-4-one, 7-[[2-O-(6-deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl]oxy]-2,3-dihydro-5-hydroxy-2-(4-hydroxyphenyl)-, (*S*)-**RN:** 10236-47-2 **MP (°C):****MW:** 580.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.928E-04	1.700E-01	6	P070	1 2 1 1 1	
8.613E-04	5.000E-01	20	P070	1 2 1 1 1	
1.361E-03	7.900E-01	35	P070	1 2 1 1 1	
3.376E-03	1.960E+00	45	P070	1 2 1 1 2	
1.233E-02	7.160E+00	55	P070	1 2 1 1 2	
7.271E-02	4.221E+01	65	P070	1 2 1 1 2	
1.864E-01	1.082E+02	75	P070	1 2 1 1 2	

4470. C₂₇H₃₃N₃O₈

Rolutetraacycline

N-(1-Pyrrolidinylmethyl)tetracycline

Syntetrin

Tetraverin

Synotodecin

RN: 751-97-3 **MP (°C):** 162dec**MW:** 527.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>3.79E-02	>2.00E+01	21	M044	2 0 2 2 0	

4471. C₂₇H₃₄O₃

Testosterone phenylacetate

Androst-4-en-3-one, 17-[(phenylacetyl)oxy]-, (17 β)-**RN:** 5704-03-0 **MP (°C):****MW:** 406.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.206E-05	8.970E-03	25	L342	1 0 1 1 2	
2.188E-05	8.895E-03	ns	R427	0 0 0 0 0	

4472. C₂₇H₃₄O₁₀

Cortisone tricarballylate

RN: **MP (°C):****MW:** 518.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.350E-04	7.000E-02	25	M023	1 0 2 1 0	

4473. C₂₇H₃₆N₂O₄

Repaglinide

RN: 135062-02-1 **MP (°C):**
MW: 452.60 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.988E-04	8.999E-02	25	M448	0 0 0 0 0	Intrinsic, EFG

4474. C₂₇H₃₈N₂O₆*p*-Ureidophenyl prostaglandin E2

RN: **MP (°C):**
MW: 486.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-05	1.363E-02	25	A066	1 0 1 1 1	

4475. C₂₇H₃₈O₃

Norethindrone heptanoate

RN: **MP (°C):**
MW: 410.60 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.468E-07	6.026E-05	25	L078	1 0 1 2 2	

4476. C₂₇H₄₀N₂O₆*p*-Ureidophenyl prostaglandin F2 α

RN: **MP (°C):**
MW: 488.63 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.900E-05	3.372E-02	25	A066	1 0 1 1 1	

4477. C₂₇H₄₀O₆

Hydrocortisone tebutate

Hydrocortisone-21-hexanoate

Hydrocortisone-21-caproate

RN: 508-96-3 **MP (°C):** 168
MW: 460.62 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.083E-06	1.420E-03	25	H098	1 0 2 0 2	
3.083E-06	1.420E-03	25	H320	0 0 0 0 0	
3.060E-06	1.409E-03	25	H320	0 0 0 0 0	

4478. C₂₇H₄₂Cl₂N₂O₆

α-Chloramphenicol palmitate

β-Chloramphenicol palmitate

Chloramphenicol palmitate

RN: 530-43-8 **MP (°C):** 359**MW:** 561.55 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.100E-08	6.177E-06	20	M006	2 2 1 2 1	
8.500E-08	4.773E-05	20	M006	2 2 1 2 1	
1.500E-08	8.423E-06	25	M006	2 2 1 2 1	
9.600E-08	5.391E-05	25	M006	2 2 1 2 1	
7.123E-06	4.000E-03	28	R004	0 0 0 0 0	
1.800E-08	1.011E-05	29	M006	2 2 1 2 1	
1.440E-07	8.086E-05	29	M006	2 2 1 2 2	
2.700E-08	1.516E-05	32	M006	2 2 1 2 1	
2.600E-07	1.460E-04	32	M006	2 2 1 2 2	
3.100E-08	1.741E-05	35	M006	2 2 1 2 1	
3.800E-07	2.134E-04	35	M006	2 2 1 2 2	

4479. C₂₇H₄₂N₄O₇.0.3H₂O

2'-(2-Heptanoyl-2-hexanyl-acetyl)-6-methoxypurine arabinoside (0.3 hydrate)

RN: 145913-52-6 **MP (°C):****MW:** 540.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.990E-04	1.615E-01	37	C348	0 0 0 0 0	pH 7.00

4480. C₂₇H₄₂O₃

Diosgenin

(25*R*)-Spirost-5-en-3β-ol**RN:** 512-04-9 **MP (°C):** 204**MW:** 414.63 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.824E-08	2.000E-05	25	L033	1 0 2 1 0	

4481. C₂₇H₄₂O₃

Nandrolone nonanoate

RN: **MP (°C):****MW:** 414.63 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.233E-06	9.260E-04	37	C026	0 0 0 0 0	

4482. C₂₇H₄₃NO₈

N-Methylglucamine testosterone

17-β-(4-Androsten-3-one)-N-methyl-N-1-(1-desoxyglucosyl) carbamate

RN: MP (°C): 183–185

MW: 509.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.633E-05	4.400E-02	25	L009	1 0 0 1 1	

4483. C₂₇H₄₄N₄O₆

2'-Hexadecyl-6-methoxypurine arabinoside

RN: 145913-43-5 MP (°C): 97–99

MW: 520.67 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-05	9.893E-03	37	C348	0 0 0 0 0	pH 7.00

4484. C₂₇H₄₄O

Vitamin D3

Cholecalciferol

Activated 7-dehydrocholesterol

Oleovitamin D3

RN: 67-97-0 MP (°C): 85

MW: 384.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<5.98E-04	<2.30E-01	25	P312	0 0 0 0 0	

4485. C₂₇H₅₈O₂P₂bis(Di-*n*-hexyl-phosphinyl)propane

HDPP

RN: 2896-56-2 MP (°C):

MW: 476.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.727E-04	1.300E-01	0	O002	2 0 2 2 0	EFG
1.154E-04	5.500E-02	15	O002	2 0 2 2 0	EFG
3.566E-05	1.700E-02	25	O002	2 0 2 2 0	

4486. C₂₈H₂₉F₂N₃O

Pimozide

2-Benzimidazolinone, 1-[1-[4,4-bis(*p*-fluorophenyl)butyl]-4-piperidyl]-

Orap

RN: 2062-78-4 **MP (°C):****MW:** 461.56 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.283E-06	2.900E-03	30	P044	0 0 0 0 0	

4487. C₂₈H₃₁FN₄O

Astemizole

1-((4-Fluorophenyl)-methyl)-*N*-(1-(2-(4-methoxyphenyl)ethyl)-4-piperidinyl)-1H-benzimidazol-2-amine

Hismanal

RN: 68844-77-9 **MP (°C):****MW:** 458.58 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	3.210E-01	30	A417	0 0 0 0 0	pH 5.8
3.700E-03	1.697E+00	30	A417	0 0 0 0 0	pH 3.8

4488. C₂₈H₃₆O₃

Testosterone phenyl propionate

Androst-4-en-3-one, 17-(1-oxo-3-phenylpropoxy)-, (17 β)-**RN:** 1255-49-8 **MP (°C):****MW:** 420.60 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.350E-06	2.250E-03	25	L342	1 0 1 1 2	

4489. C₂₈H₃₆O₁₅

Neohesperidin dihydrochalcone

1-Propanone, 1-[4-[[2-*O*-(6-deoxy-a-L-mannopyranosyl)-b-D-glucopyranosyl]oxy]-2,6-dihydroxyphenyl]-3-(3-hydroxy-4-methoxyphenyl)-Glucopyranoside, 3,5-dihydroxy-4-(3-hydroxy-4-methoxyhydrocinnamoyl)phenyl 2-*O*-(6-deoxy-a-L-mannopyranosyl)-, b-D-Glucopyranoside, 3,5-dihydroxy-4-(3-hydroxy-4-methoxyhydrocinnamoyl)phenyl 2-*O*-a-L-rhamnopyranosyl-

Neohesperidin DHC

NHDC

RN: 20702-77-6 **MP (°C):****MW:** 612.59 **BP (°C):** 927.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.530E-06	4.000E-03	rt	B417	0 0 1 2 1	

4490. C₂₈H₃₈N₆O₁₁S

Sildenafil citrate

1-[[3-(6,7-Dihydro-1-methyl-7-oxo-3-propyl-1H-pyrazolo [4,3-d]pyrimidin-5-yl)-4-ethoxyphenyl] sulfonyl]-4-methylpiperazine citrate

Viagra

RN: 171599-83-0 MP (°C):

MW: 666.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.231E-03	3.488E+00	ns	S469	0 0 0 0 0	

4491. C₂₈H₃₉NO₆*p*-Acetamidophenyl prostaglandin E2

RN: MP (°C):

MW: 485.63 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.400E-05	2.622E-02	25	A066	1 0 1 1 1	

4492. C₂₈H₃₉NO₆

2-Oxo-5-indolinyl prostaglandin F2α

Prosta-5,13-dien-1-oic acid, 9,11,15-trihydroxy-, 2,3-dihydro-2-oxo-1H-indol-5-yl ester,
(5Z,9α,11α,13E,15S)-

RN: 74973-22-1 MP (°C):

MW: 485.63 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.000E-05	2.914E-02	25	A066	1 0 1 1 1	

4493. C₂₈H₃₉N₃O₆α-Semicarbazono-*p*-tolyl prostaglandin E2

RN: MP (°C):

MW: 513.64 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.500E-06	1.284E-03	25	A066	1 0 1 1 1	

4494. C₂₈H₄₀FNO₁₁.H₂O

Glucosamine 9-α-fluorohydrocortisome (monohydrate)

21-(9-α-Fluoro-11α, 17α-dihydroxy-4-pregnene-3,20-dione)-N-2-(2-desoxyglucosyl) carbamate

RN: MP (°C): 176-178

MW: 603.64 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.964E-04	3.600E-01	25	L009	1 0 0 1 1	

4495. C₂₈H₄₁N₃O₆ α -Semicarbazono-*p*-tolyl prostaglandin F2 α

RN: MP (°C):

MW: 515.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.600E-05	8.250E-03	25	A066	1 0 1 1 1	

4496. C₂₈H₄₂FNO₁₁.H₂OGlucamine 9- α -fluorohydrocortisome (monohydrate)

RN: MP (°C): 105–110

MW: 605.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.456E-03	2.699E+00	25	L009	1 0 0 1 1	

4497. C₂₈H₄₂O₆

Hydrocortisone heptanoate

Hydrocortisone-21-heptanoate

RN: MP (°C):

MW: 474.64 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.082E-06	9.880E-04	25	H098	1 0 2 0 2	
2.082E-06	9.880E-04	25	H320	0 0 0 0 0	
2.060E-06	9.778E-04	25	H320	0 0 0 0 0	

4498. C₂₈H₄₄O₃

Nandrolone decanoate

Deca-durabolin

Norandrostenolone decanoate

RN: 360-70-3 MP (°C):

MW: 428.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.549E-06	6.640E-04	37	C026	0 0 0 0 0	

4499. C₂₈H₄₆O₄Di-*n*-decyl phthalate

RN: 84-77-5 MP (°C):

MW: 446.68 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.388E-07	3.300E-04	24	H116	2 1 0 0 2	

4500. C₂₈H₄₆O₄

Diisodecyl phthalate

RN: 26761-40-0

MP (°C):

MW: 446.68

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.269E-07	2.800E-04	24	H116	2 1 0 0 2	

4501. C₂₈H₆₀O₂P₂bis(Di-*n*-hexyl-phosphinyl)butane

HDPB

RN: 2785-35-5

MP (°C):

MW: 490.74

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.627E-04	1.780E-01	0	O002	2 0 2 2 0	EFG
1.284E-04	6.300E-02	15	O002	2 0 2 2 0	EFG
4.076E-05	2.000E-02	25	O002	2 0 2 2 0	

4502. C₂₉H₂₀N₂O₄

1,4-Dibenzoylaminoanthraquinone

Benzamide, *N,N'*-(9,10-dihydro-3-methyl-9,10-dioxo-1,8-anthracenediyl)bis

RN: 4627-15-0

MP (°C):

MW: 460.49

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.200E-05	1.013E-02	50	G077	1 0 0 0 1	

4503. C₂₉H₂₇N₅O₄*m*-Nitrophenyldiantipyrylmethane*m*-NPhDAM

RN: 1606-53-7

MP (°C):

MW: 509.57

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.887E-05	3.000E-02	20	P054	0 0 0 0 0	

4504. C₂₉H₂₇N₅O₄*o*-Nitrophenyldiantipyrylmethane*o*-NPhDAM

RN: 14957-18-7

MP (°C):

MW: 509.57

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-05	2.000E-02	20	P054	0 0 0 0 0	

4505. C₂₉H₂₇N₅O₄

p-Nitrophenyldiantipyrylmethane
p-NPhDAM

RN: 55774-19-1 **MP (°C):**
MW: 509.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.925E-05	2.000E-02	20	P054	0 0 0 0 0	

4506. C₂₉H₂₈N₄O₂

Phenyldiantipyrylmethane
 PhDAM

RN: 1861-84-3 **MP (°C):**
MW: 464.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.165E-04	2.399E-01	20	P054	0 0 0 0 0	

4507. C₂₉H₂₈N₄O₃

o-Hydroxylphenyldiantipyrylmethane
o-HPhDAM

RN: 1606-55-9 **MP (°C):**
MW: 480.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.08E-05	<1.00E-02	20	P054	0 0 0 0 0	

4508. C₂₉H₂₈N₄S₂

Phenyldithiopyrylmethane

3H-Pyrazole-3-thione, 4,4'-(phenylmethylene)bis[1,2-dihydro-1,5-dimethyl-2-phenyl-

RN: 74713-68-1 **MP (°C):** 160
MW: 496.70 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-05	2.086E-02	ns	D087	0 2 0 0 1	

4509. C₂₉H₃₂O₁₃

Etoposide

4'-Demethylepipodophyllotoxin ethylidene-β-D-glucoside

Vepesid

VP-16

RN: 33419-42-0 **MP (°C):** 236–251**MW:** 588.57 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.945E-04	1.145E-01	25	S466	0 0 0 0 0	
3.398E-04	2.000E-01	ns	D347	0 0 0 0 0	
3.388E-04	1.994E-01	ns	R427	0 0 0 0 0	

4510. C₂₉H₃₅NO₂

Mifepristone

RU-486

RN: 84371-65-3 **MP (°C):****MW:** 429.61 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.105E-06	4.748E-04	22.5	B440	0 0 0 0 0	

4511. C₂₉H₃₆N₄O₂

Hexyldiantipyrylmethane

HDAM

RN: 7660-44-8 **MP (°C):****MW:** 472.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.230E-05	1.999E-02	20	P054	0 0 0 0 0	
4.232E-05	2.000E-02	20	P054	0 0 0 0 0	

4512. C₂₉H₃₆N₄S₂

Hexyldithiopyrylmethane

3H-Pyrazole-3-thione, 4,4'-heptylidenebis[1,2-dihydro-1,5-dimethyl-2-phenyl-

RN: 74713-69-2 **MP (°C):** 169**MW:** 504.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-05	2.070E-02	0	D087	0 2 0 0 1	

4513. C₂₉H₃₈Cl₂N₂O₃

3β-Hydroxy-13α-amino-13,17-seco-5α-androstan-17-oic-13,17-lactam-4-N,N-bis-(chloroethyl) amino phenyl-acetate

RN: MP (°C):
MW: 533.54 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.186E-07	1.700E-04	25	P022	0 0 0 0 0	
3.599E-07	1.920E-04	30	P022	0 0 0 0 0	
4.517E-07	2.410E-04	44	P022	0 0 0 0 0	
6.110E-07	3.260E-04	73	P022	0 0 0 0 0	

4514. C₂₉H₃₈O₃

Testosterone phenylbutyrate

RN: MP (°C):
MW: 434.62 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.681E-06	1.600E-03	25	L342	1 0 1 1 2	

4515. C₂₉H₄₀N₂O₄

Emetine

Emetan, 6',7',10,11-tetramethoxy-
NSC 33669

RN: 483-18-1 MP (°C): 74
MW: 480.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-03	9.613E-01	15	K059	2 2 2 0 0	
2.078E-03	9.990E-01	c	D004	0 0 0 0 0	

4516. C₂₉H₄₂O₆

Cortisone caprylate

RN: MP (°C):
MW: 486.65 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.110E-06	2.000E-03	25	M023	1 0 2 1 0	

4517. C₂₉H₄₄FNO₁₁.H₂O*N*-Methylglucamine 9- α -fluorohydrocortisone (monohydrate)21-(9- α -Fluoro-11 β , 17 α -dihydroxy-4-pregnene-3,20-dione)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate

RN: **MP (°C):** 120
MW: 619.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.358E-03	3.940E+00	25	L009	1 0 0 1 1	

4518. C₂₉H₄₄O₁₂

Oubain

 γ -Strophanthin

Ouabain

Quabain

RN: 630-60-4 **MP (°C):** 185
MW: 584.67 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.223E-02	1.300E+01	25	P312	0 0 0 0 0	
1.693E-02	9.901E+00	c	D004	0 0 0 0 0	
2.851E-01	1.667E+02	h	D004	0 0 0 0 0	

4519. C₂₉H₄₆N₄O₇.0.4H₂O

2'-(2-Octanoyl-2-heptyanyl-acetyl)-6-methoxypurine arabinoside (0.4 hydrate)

RN: 145913-53-7 **MP (°C):**
MW: 569.92 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.810E-05	1.601E-02	37	C348	0 0 0 0 0	pH 7.00

4520. C₂₉H₄₆O₃

Nandrolone undecanoate

RN: **MP (°C):**
MW: 442.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.360E-06	6.020E-04	37	C026	0 0 0 0 0	

4521. C₂₉H₅₀O₂

Vitamin E

α-Tocopherol

RN: 59-02-9

MP (°C):

MW: 430.72

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.833E-05	2.082E-02	33	D404	2 1 2 2 2	
4.852E-05	2.090E-02	33	D404	2 1 2 2 2	

4522. C₃₀H₂₈N₄O₃

Benzoyldiantipyrylmethane

BenzDAM

RN: 55774-17-9 MP (°C):

MW: 492.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.03E-05	<1.00E-02	20	P054	0 0 0 0 0	

4523. C₃₀H₃₀N₂₀O₁₀

Cucurbit[5]uril

RN: 259886-49-2 MP (°C):

MW: 830.70 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-04	3.406E-01	25	B424	1 0 1 2 2	

4524. C₃₀H₃₄O₁₃

Picrotoxin

Picrotoxine

RN: 124-87-8 MP (°C):

MW: 602.60 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.964E-03	2.991E+00	20	D041	1 0 0 0 0	
6.776E-03	4.083E+00	rt	D021	0 0 1 1 1	

4525. C₃₀H₄₈O₃

β-Boswellic acid

RN: MP (°C):

MW: 456.72 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-02	7.764E+00	ns	R422	0 0 0 0 0	

4526. C₃₀H₄₈O₁₂

Periplocin

Card-20(22)-enolide, 3-[(2,6-dideoxy-4-O-β-D-glucopyranosyl-3-O-methyl-β-D-ribo-hexopyranosyl)oxy]-5,14-dihydroxy-, (3β,5β)-

Periplocoside

RN: 13137-64-9 MP (°C): 205

MW: 600.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.321E-02	7.937E+00	c	D004	0 0 0 0 0	

4527. C₃₁H₃₃N₅O₂*p*-Dimethylaminophenylantipyrilmethane*p*-DMAPhDAM

RN: 2088-76-8 MP (°C):

MW: 507.64 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.576E-04	7.999E-02	20	P054	0 0 0 0 0	

4528. C₃₁H₃₈N₂O₁₁

Dihydroronovobiocin

Benzamide, *N*-[7-[[3-O-(aminocarbonyl)-6-deoxy-5-C-methyl-4-O-methyl-β-L-lyxohexopyranosyl]oxy]-4-hydroxy-8-methyl-2-oxo-2H-1-benzopyran-3-yl]-4-hydroxy-3-(3-methylbutyl)-

RN: 29826-16-2 MP (°C):

MW: 614.66 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.928E-04	1.800E-01	28	A038	2 0 1 1 2	

4529. C₃₁H₄₂FNO₁₂.H₂O

Glucosamine triamcinolone acetonide (monohydrate)

21-(9-α-Fluoro-11β-hydroxy-16α, 17α-isopropylidenedioxy-1,4-pregnadien-3,20-dione)-*N*-2-(2-desoxyglucosyl) carbamate

RN: MP (°C): 250–255

MW: 657.69 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.717E-04	3.760E-01	25	L009	1 0 0 1 1	

4530. C₃₁H₄₄FNO₁₂·H₂O

Glucaminetriamcinolone acetonide (monohydrate)

21-(9- α -Fluoro-11 β -hydroxy-16 α , 17 α -isopropylidenedioxy-1,4-pregnadien-3,20-dione)-N-1-(1-desoxyglucosyl) carbamate**RN:** MP (°C): 150**MW:** 659.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.366E-03	3.540E+00	25	L009	1 0 0 1 1	

4531. C₃₁H₄₄N₂O₇

N-Acetyl-L-tyrosinamide prostaglandin E2

RN: MP (°C):**MW:** 556.71 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.700E-04	9.464E-02	25	A066	1 0 1 1 1	

4532. C₃₁H₄₆N₂O₇N-Acetyl-L-tyrosinamide prostaglandin F2 α **RN:** MP (°C):**MW:** 558.72 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-04	7.822E-02	25	A066	1 0 1 1 1	

4533. C₃₁H₄₈O₁₂

Strophanthin

k-Strophanthin

RN: 11005-63-3 MP (°C): 179**MW:** 612.72 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.709E-02	2.273E+01	25	D004	0 0 0 0 0	

4534. C₃₂H₃₂O₁₄

Chartreusin

Lambdamycin

NSC 5159

Antibiotic X 465A

RN: 6377-18-0 MP (°C): 246–249**MW:** 640.60 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.342E-05	1.500E-02	25	P067	0 0 0 0 0	

4535. C₃₂H₃₇NO₅S

Dextropropoxyphene napsylate

Darvocet N-50

Darvocet N-100

Darvon-N

RN: 17140-78-2 **MP (°C):****MW:** 547.72 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.556E-03	1.400E+00	22	N319	0 0 0 0 0	

4536. C₃₂H₄₀BrN₅O₅

Bromocriptine

2-Bromo- α -ergocryptine

Parlodel

Kripton

(5' α)-2-Bromo-12'-hydroxy-2'-(1-methylethyl)-5'-(2-methylpropyl)ergotaman-3',6',18-trione**RN:** 25614-03-3 **MP (°C):****MW:** 654.62 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.162E-06	2.070E-03	ns	R427	0 0 0 0 0	

4537. C₃₂H₄₁NO₂

Terfenadine

Seldane

Teldane

RN: 50679-08-8 **MP (°C):****MW:** 471.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.056E-10	9.700E-08	25	A412	1 0 2 2 1	
		amb	L434	0 0 0 0 0	
2.138E-07	1.008E-04	ns	R427	0 0 0 0 0	

4538. C₃₂H₄₅N₃O₄S

Nelfinavir mesylate

Nelfinavir

NFV

Viracept

RN: 159989-65-8 **MP (°C):****MW:** 567.80 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.925E-03	4.500E+00	ns	W424	0 0 0 0 0	

4539. C₃₂H₄₅N₃O₄S

Nelfinavir

(3S,4aS,8aS)-N-(1,1-Dimethylethyl)decahydro-2-[(2R,3R)-2-hydroxy-3-[(3-hydroxy-2-methylbenzoyl)amino]-4-(phenylthio)butyl]-3-isoquinolinecarboxamide

RN: 159989-64-7 **MP (°C):****MW:** 567.80 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.233E-02	7.000E+00	ns	A426	0 0 0 0 0	Intrinsic

4540. C₃₂H₄₆FNO₁₂·H₂O

N-Methylglucamine triamcinolone acetonide (monohydrate)

21-(9- α -Fluoro-11 β -hydroxy-16 α , 17 α -isopropylidenedioxy-1,4-pregnadien-3,20-dione)-N-methyl-N-1-(1-desoxyglucosyl) carbamate**RN:** **MP (°C):** 152**MW:** 673.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.744E-03	3.196E+00	25	L009	1 0 0 1 1	

4541. C₃₂H₄₉NO₉

Cevadine

Cevane-3,4,12,14,16,17,20-heptol, 4,9-epoxy-, 3-[(2Z)-2-methyl-2-butenoate], (3 β ,4 α ,16 β)-Veratrine**RN:** 62-59-9 **MP (°C):** 213.5**MW:** 591.75 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-03	4.734E+00	15	K059	2 2 2 0 0	

4542. C₃₂H₅₄O₄

Didodecyl phthalate

1,2-Benzenedicarboxylic acid, didodecyl ester

RN: 2432-90-8 **MP (°C):****MW:** 502.78 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.784E-07	1.400E-04	24	H116	2 1 0 0 2	

4543. C₃₃H₂₅N₃O₃

Norbormide

5-(α -Hydroxy- α -2-pyridylbenzyl)-7-(α -2-pyridylbenzylidene)-5-norbornene-2,3-dicaboximide

Shoxin

RN: 991-42-4 **MP (°C):** >160**MW:** 511.59 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.173E-04	6.000E-02	rt	M161	0 0 0 0 1	

4544. C₃₃H₃₄O₃

Norethindrone biphenyl-4-carboxylate

RN: **MP (°C):****MW:** 478.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.762E-09	3.715E-06	25	L078	1 0 1 2 2	

4545. C₃₃H₃₄O₄

Norethindrone 4-phenoxybenzoate

RN: **MP (°C):****MW:** 494.64 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.431E-07	7.079E-05	25	L078	1 0 1 2 2	

4546. C₃₃H₃₆N₄O₆

Bilirubin

21H-Biline-8,12-dipropanoic acid, 2,17-diethenyl-1,10,19,22,23,24-hexahydro-3,7,13,18-tetramethyl-1,19-dioxo-

RN: 635-65-4 **MP (°C):****MW:** 584.68 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-09	4.093E-06	18	K104	1 0 0 0 2	intrinsic

4547. C₃₃H₄₀N₂O₉

Reserpine

3,4,5-Trimethoxybenzoyl methyl reserpate

Rauwilid

Rauwiloid

RN: 50-55-5**MP (°C):****MW:** 608.69**BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-04	7.304E-02	30	L068	1 0 0 1 0	EFG
1.643E-05	1.000E-02	ns	K444	0 0 0 0 0	

4548. C₃₃H₄₁N₅O₆S₂

Kynostatin

KNI-272

4-Thiazolidinecarboxamide, *N*-(1,1-dimethylethyl)-3-[(2*S*,3*S*)-2-hydroxy-3-[(2*R*)-2-[(5-isoquinolinyloxy)acetyl]amino]-3-(methylthio)-1-oxopropyl]amino]-1-oxo-4-phenylbutyl]-, (4*R*)-**RN:** 147318-81-8 **MP (°C):****MW:** 667.85 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.289E-06	4.200E-03	25	J308	0 0 0 0 0	

4549. C₃₃H₄₅NO₉

Delphinine

Indaconitine, *N*-deethyl-3-deoxy-*N*-methyl-**RN:** 561-07-9 **MP (°C):** 198–200**MW:** 599.73 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.335E-05	2.000E-02	25	D004	0 0 0 0 0	

4550. C₃₃H₄₇NO₁₃

Natamycin

Pimafucin

RN: 7681-93-8 **MP (°C):****MW:** 665.74 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.506E-05	3.000E-02	20	B190	1 2 1 1 0	
6.159E-04	4.100E-01	21	M044	2 0 2 2 2	sic

4551. C₃₄H₃₀N₂O₆S

Pyrantel pamoate

Pirantel pamoate

Dog Wormer

Helmex

Lombriareu

Trilombrin

RN: 22204-24-6 **MP (°C):** 266–267**MW:** 594.69 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.682E-05	1.000E-02	ns	K444	0 0 0 0 0	

4552. C₃₄H₃₄N₄O₄

Protoporphyrin IX

Protoporphyrin IX

RN: 553-12-8 **MP (°C):****MW:** 562.67 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.900E-04	1.069E-01	25	C097	2 0 1 1 1	EFG

4553. C₃₄H₄₇NO₁₁

Aconitine

Acetylbenzoylaconine

RN: 302-27-2 **MP (°C):** 204**MW:** 645.75 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.691E-04	3.029E-01	25	D004	0 0 0 0 0	

4554. C₃₄H₅₀O₇

Carbenoxolone

Olean-12-en-29-oic acid, 3-(3-carboxy-1-oxopropoxy)-11-oxo-, (3β,20β)-

RN: 5697-56-3 **MP (°C):****MW:** 570.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.160E-05	6.621E-03	24	B363	0 0 0 0 0	
1.630E-05	9.304E-03	37	B363	0 0 0 0 0	

4555. C₃₄H₅₇NO₇

Glucosamine cholesterol

3-β-(5-Cholestanyl)-N-2-(2-desoxyglucosyl) carbamate

RN: MP (°C): 155–158**MW:** 591.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.530E-04	5.640E-01	25	L009	1 0 0 1 1	

4556. C₃₄H₅₈O₄

Ditridecyl phthalate

Staflex DTDP

Truflex DTDP

Hexaplas DTDP

Jayflex DTDP

Polycizer 962BPA

RN: 119-06-2 **MP (°C):****MW:** 530.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.405E-07	3.400E-04	24	H116	2 1 0 0 2	

4557. C₃₄H₆₈N₃O₈S₂

Lincomycin hexadecylsulfamate

RN: MP (°C):**MW:** 711.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.738E-04	4.080E-01	21	M044	2 0 2 2 2	

4558. C₃₅H₄₄N₂O₇p-(*p*-Acetamidobenzamido)phenyl prostaglandin E2**RN:** MP (°C):**MW:** 604.75 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-08	5.927E-05	25	A066	1 0 1 1 1	

4559. C₃₅H₄₆N₂O₇*p*-(*p*-Acetamidobenzamido)phenyl prostaglandin F2 α

RN: **MP (°C):**
MW: 606.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.800E-07	1.699E-04	25	A066	1 0 1 1 1	

4560. C₃₅H₄₇NO₉

Rhizoxin

RN: 90996-54-6 **MP (°C):**
MW: 625.77 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.918E-05	1.200E-02	25	P336	0 0 0 0 0	

4561. C₃₅H₆₁NO₇*N*-Methylglucamine cholesterol3- β -(5-Cholestanyl)-*N*-methyl-*N*-1-(1-desoxyglucosyl) carbamate

RN: **MP (°C):** 131–133
MW: 607.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.842E-04	1.120E-01	25	L009	1 0 0 1 1	

4562. C₃₆H₄₇N₂O₇*N*-Benzoyl-L-tyrosinamide prostaglandin E2

RN: **MP (°C):**
MW: 619.79 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.700E-07	2.913E-04	25	A066	1 0 1 1 1	

4563. C₃₆H₄₇N₅O₄

Indinavir sulfate

Crixivan

IDV

Indinavir

Indinavir sulfate

MK-639

RN: 157810-81-6 **MP (°C):****MW:** 613.81 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.63E-01	>1.00E+02	ns	W424	0 0 0 0 0	

4564. C₃₆H₄₇N₅O₄

Indinavir

2,3,5-Trideoxy-N-[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]-5-[(2S)-2-[[((1,1-dimethylethyl)amino]carbonyl]-4-(3-pyridinylmethyl)-1-piperazinyl]-2-(phenylmethyl)-D-erythro-pentonamide
N-(2-hydroxy-1(S)-indanyl)-2-(phenylmethyl)-4(S)-hydroxy-5-[1-[4-(3-pyridylmethyl)-2(S)-(N-tert-butylcarbamoyl)piperazinyl]]pentanamide

RN: 150378-17-9 **MP (°C):****MW:** 613.81 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.140E-04	7.000E-02	ns	A426	0 0 0 0 0	Intrinsic

4565. C₃₆H₄₉N₂O₇N-Benzoyl-L-tyrosinamide prostaglandin F2 α **RN:** **MP (°C):****MW:** 621.80 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-06	1.119E-03	25	A066	1 0 1 1 1	

4566. C₃₆H₅₆O₁₄

Digitalalin

Card-20(22)-enolide, 3-[(6-deoxy-4-O- β -D-glucopyranosyl-3-O-methyl- β -D-galactopyranosyl)oxy]-14,16-dihydroxy-, (3 β ,5 β ,16 β)-

Digitalatinum verum

RN: 752-61-4 **MP (°C):** 229**MW:** 712.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.401E-03	9.990E-01	25	D004	0 0 0 0 0	

4567. C₃₆H₅₇N₇O₁₀S

L-Histidinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-N-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[(2-sulfoethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-, [1S-[1R*,2R*,4(R*)]]-

RN: 100902-06-5 **MP (°C):**
MW: 779.96 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>1.10E-02	>8.58E+00	ns	B425	0 0 0 1 0	

4568. C₃₆H₅₈N₈O₇

L-Leucinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-histidyl-(3S,4S)-4-amino-3-hydroxy-6-methylheptanoyl-N-(2-aminoethyl)-

L-Histidinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-N-[4-[[1-[(2-aminoethyl)amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 105192-87-8 **MP (°C):**
MW: 714.91 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.900E-03	3.503E+00	ns	B425	0 0 0 1 0	pH 7.4

4569. C₃₆H₆₀O₂

Vitamin A palmitate

Retinol, hexadecanoate

Retinyl palmitate

RN: 79-81-2 **MP (°C):**
MW: 524.88 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.000E-07	2.624E-04	25	P343	0 0 0 0 0	
1.905E-05	1.000E-02	ns	K444	0 0 0 0 0	

4570. C₃₆H₆₀O₃₀

α-Cyclodextrin

β-Hexaamylose

(C₆H₁₀O₅)₆

α-Dextrin

RN: 10016-20-3 **MP (°C):**
MW: 972.86 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.345E-02	9.091E+01	20	F186	1 2 1 1 1	
2.409E-02	2.344E+01	20	P048	1 0 1 1 1	sic
1.118E-01	1.088E+02	23.7	J305	0 0 0 0 0	
1.204E-01	1.171E+02	23.7	J305	0 0 0 0 0	
1.460E-01	1.420E+02	25	B396	0 0 0 0 0	

(continued)

4570. C₃₆H₆₀O₃₀ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.490E-01	1.450E+02	25	L432	0 0 0 0 0	
1.800E-01	1.751E+02	25	O321	0 0 0 0 0	
1.331E-01	1.295E+02	25	S462	0 0 0 0 0	
1.211E-01	1.178E+02	25.0	J305	0 0 0 0 0	
1.318E-01	1.282E+02	25.0	J305	0 0 0 0 0	
1.678E-01	1.632E+02	30.0	J305	0 0 0 0 0	
1.501E-01	1.460E+02	30.0	J305	0 0 0 0 0	
1.696E-01	1.650E+02	33.0	J305	0 0 0 0 0	
1.912E-01	1.860E+02	33.0	J305	0 0 0 0 0	
2.161E-01	2.102E+02	35.0	J305	0 0 0 0 0	
1.885E-01	1.834E+02	35.0	J305	0 0 0 0 0	
2.331E-01	2.268E+02	38.0	J305	0 0 0 0 0	
2.023E-01	1.968E+02	38.0	J305	0 0 0 0 0	
2.100E-01	2.043E+02	40	O321	0 0 0 0 0	
2.171E-01	2.112E+02	40.0	J305	0 0 0 0 0	
2.532E-01	2.463E+02	40.0	J305	0 0 0 0 0	
2.229E-01	2.169E+02	42.0	J305	0 0 0 0 0	
2.616E-01	2.545E+02	42.0	J305	0 0 0 0 0	
2.677E-01	2.604E+02	43.0	J305	0 0 0 0 0	
2.283E-01	2.221E+02	43.0	J305	0 0 0 0 0	
2.492E-01	2.424E+02	45.0	J305	0 0 0 0 0	
2.982E-01	2.901E+02	45.0	J305	0 0 0 0 0	
3.397E-01	3.305E+02	48.0	J305	0 0 0 0 0	
2.773E-01	2.698E+02	48.0	J305	0 0 0 0 0	
4.700E-01	4.572E+02	55	O321	0 0 0 0 0	
1.302E-01	1.266E+02	ns	M335	0 0 2 0 1	
1.490E-01	1.450E+02	rt	F041	0 2 2 0 2	

4571. C₃₆H₇₂N₃O₈S₂

Lincomycin octadecylsulfamate

RN: MP (°C):

MW: 739.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.897E-04	2.880E-01	21	M044	2 0 2 2 2	

4572. C₃₆H₇₄

n-Hexatriacontane

Hexatriacontane

RN: 630-06-8 MP (°C): 75.0

MW: 506.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.353E-09	1.700E-06	25	B069	1 0 1 1 1	
4.122E-09	2.090E-06	ns	B033	0 0 0 0 2	
4.122E-09	2.090E-06	ns	B033	0 0 0 0 0	

4573. C₃₇H₄₈N₆O₅S₂

Ritonavir

ABT-538

Norvir

Ritonavir

RN: 155213-67-5 **MP (°C):****MW:** 720.96 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.935E-06	5.000E-03	ns	A426	0 0 0 0 0	intrinsic
1.387E-05	1.000E-02	ns	K444	0 0 0 0 0	
~1.39E+00	~9.99E+02	ns	W424	0 0 0 0 0	

4574. C₃₇H₆₇NO₁₃.2H₂O

Erythromycin (dihydrate)

RN: 114-07-8 **MP (°C):****MW:** 769.98 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.857E-04	5.280E-01	30	F310	1 0 2 2 2	
4.922E-04	3.790E-01	40	F310	1 0 2 2 2	
4.377E-04	3.370E-01	50	F310	1 0 2 2 2	
4.143E-04	3.190E-01	60	F310	1 0 2 2 2	
4.598E-04	3.540E-01	70	F310	1 0 2 2 2	
5.688E-04	4.380E-01	80	F310	1 0 2 2 2	

4575. C₃₈H₅₀N₆O₅

Squinavir

Butanediamide, *N*1-[*(1S,2R)*-3-[(3*S*,4*aS*,8*aS*)-3-[[[(1,1-dimethylethyl)amino]carbonyl]octahydro-2-(1*H*)-isoquinolinyl]-2-hydroxy-1-(phenylmethyl)propyl]-2-[(2-quinolinylcarbonyl)amino]-

Squinavir mesylate

Fortovase

Invirase

(S)-*N*-(*aS*)-*a*-[(1*R*)-2-[(3*S*,4*aS*,8*aS*)-3-(*tert*-Butylcarbamoyl)octahydro-2(*1H*)-isoquinolyl]-1-hydroxyethyl]phenethyl]-2-quinaldamidosuccinamide**RN:** 127779-20-8 **MP (°C):****MW:** 670.86 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.336E-05	3.580E-02	25	B431	1 0 1 1 0	
8.198E-05	5.500E-02	25	C437	0 0 0 0 0	Average
3.309E-03	2.220E+00	ns	W424	0 0 0 0 0	

4576. C₃₈H₆₀N₈O₉

Butanoic acid, N4-[N-[4-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-2,4-diamino-

RN: 115511-05-2 **MP (°C):**
MW: 772.95 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-03	1.778E+00	ns	B425	0 0 0 1 0	pH 7.4

4577. C₃₈H₆₉NO₁₃

Clarithromycin

Biaxin

A-56268

TE-031

RN: 81103-11-9 **MP (°C):** 218.5
MW: 747.97 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.330E-04	9.948E-02	20	N334	0 0 0 0 0	EFG
1.089E-04	8.145E-02	37	N334	0 0 0 0 0	EFG
4.893E-05	3.660E-02	50	N334	0 0 0 0 0	EFG

4578. C₄₀H₅₁NO₁₄

Streptovaricin C

Streptovaricin

RN: 1404-74-6 **MP (°C):** 189
MW: 769.85 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.604E-03	1.235E+00	21	M044	2 0 2 2 2	

4579. C₄₀H₅₈N₈O₇

L-Histidinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-N-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[[2-pyridinylmethyl]amino]carbonyl]butyl]amino]-4-oxobutyl]-

RN: 87691-49-4 **MP (°C):**
MW: 762.96 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.800E-04	1.373E-01	ns	B425	0 0 0 1 0	pH 7.4

4580. C₄₀H₅₈N₈O₇

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-1-(2-methylpropyl)-4-[[3-methyl-1-[(4-pyridinylmethyl)amino]carbonyl]butyl]amino]-4-oxobutyl]-

RN: 87691-50-7 **MP (°C):**
MW: 762.96 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-04	2.594E-01	ns	B425	0 0 0 1 0	pH 7.4

4581. C₄₀H₅₈N₈O₈

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[[(1-oxido-4-pyridinyl)methyl]amino]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100902-03-2 **MP (°C):**
MW: 778.96 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.200E-03	3.272E+00	ns	B425	0 0 0 1 0	pH 7.4

4582. C₄₁H₅₉N₇O₇

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[2-hydroxy-4-[[3-methyl-1-[[[(phenylmethyl)amino]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-

RN: 109585-11-7 **MP (°C):**
MW: 761.97 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<7.62E-03	ns	B425	0 0 0 1 0	pH 7.4

4583. C₄₁H₆₁N₈O₇

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[2-amino-2-(2-pyridinyl)ethyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100901-99-3 **MP (°C):**
MW: 792.00 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.000E-04	3.168E-01	ns	B425	0 0 0 1 0	pH 7.4

4584. C₄₁H₆₄O₁₃

Digitoxin

(3 β ,5 β)-3-[(2,6-Dideoxy- β -D-ribo-hexopyranosyl-(1 \rightarrow 4)-O-2,6-dideoxy- β -D-ribo-hexopyranosyl-(1 \rightarrow 4)-2,6-dideoxy- β -D-ribo-hexopyranosyl)oxy]-14-hydroxycard-20(22)-enolide

Crystodigin

Digifortis

RN: 71-63-6

MP (°C): 256

MW: 764.96

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.307E-05	1.000E-02	20	J010	1 0 0 0 0	
5.098E-06	3.900E-03	25	M301	1 1 2 2 1	anhydrate
2.000E-05	1.530E-02	30	O321	0 0 0 0 0	
2.222E-05	1.700E-02	30	O321	0 0 0 0 0	
1.447E-05	1.107E-02	37	C303	2 2 2 2 2	average of 3
3.255E-06	2.490E-03	37	M301	1 1 2 2 1	anhydrate
1.300E-05	9.944E-03	ns	M070	0 0 0 0 1	
9.151E-06	7.000E-03	ns	N302	0 2 1 2 0	

4585. C₄₁H₆₄O₁₄

Digoxin

3 β -((2,6-Dideoxy- β -D-ribo-hexopyranosyl-(1 \rightarrow 4)-O-2,6-dideoxy- β -D-ribo-hexopyranosyl-(1 \rightarrow 4)-2,6-dideoxy- β -D-ribo-hexopyranosyl)oxy)-12 β ,14-dihydroxy-5 β -card-20(22)-enolide

Lanoxicaps

Lanoxin

RN: 20830-75-5

MP (°C): 260

MW: 780.96

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.253E-04	9.789E-02	25	F010	2 1 2 2 2	Swiss micron
6.786E-05	5.300E-02	25	F010	2 1 2 2 2	
7.375E-05	5.760E-02	25	F010	2 1 2 2 2	Swiss standard
8.297E-05	6.480E-02	25	F010	2 1 2 2 2	
1.000E-04	7.810E-02	25	H066	1 0 0 0 0	EFG
3.585E-05	2.800E-02	25	M301	1 1 2 2 1	
3.675E-05	2.870E-02	25	N301	2 0 2 2 2	
3.841E-05	3.000E-02	27	E052	2 0 2 2 0	EFG
3.585E-05	2.800E-02	30	O321	0 0 0 0 0	
4.000E-05	3.124E-02	30	O321	0 0 0 0 0	
6.312E-05	4.930E-02	37	C303	2 2 2 2 2	average of 6
3.457E-05	2.700E-02	37	M301	1 1 2 2 1	
3.483E-05	2.720E-02	37	N301	2 0 2 2 2	
4.443E-05	3.470E-02	37	R009	1 0 0 0 2	
2.817E-05	2.200E-02	100	D027	1 2 0 0 1	
1.268E-03	9.900E-01	amb	L434	0 0 0 0 0	
7.363E-06	5.750E-03	ns	F037	0 0 2 0 2	mp 225.5 C
8.963E-06	7.000E-03	ns	F037	0 0 2 0 2	mp 225.5 C
5.570E-06	4.350E-03	ns	F037	0 0 2 0 2	mp 228.5 C

(continued)

4585. C₄₁H₆₄O₁₄ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.915E-06	5.400E-03	ns	F037	0 0 2 0 2	mp 235.5 C
1.280E-05	1.000E-02	ns	K444	0 0 0 0 0	
4.097E-05	3.200E-02	ns	N302	0 2 1 2 1	
5.900E-05	4.608E-02	rt	J034	0 0 0 0 0	

4586. C₄₁H₆₄O₁₄

Gitoxin

Anhydrogitalin

Pseudodigitoxin

Digitalin

RN: 4562-36-1 MP (°C):

MW: 780.96 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-06	2.343E-03	ns	M070	0 0 0 0 0	

4587. C₄₁H₆₇NO₁₅

Troleandomycin

Triacetyloleandomycin

RN: 2751-09-9 MP (°C):

MW: 813.99 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.071E-04	2.500E-01	28	A038	2 0 1 1 1	

4588. C₄₁H₆₈N₈O₉

L-Histidinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-N-[4-[[1-[[3-[bis(2-hydroxyethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 87691-52-9 MP (°C):

MW: 817.05 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.300E-03	3.513E+000	ns	B425	0 0 0 1 0	

4589. C₄₂H₅₉N₇O₉

Glycine, *N*-[*N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-D-2-phenyl-

RN: 115511-06-3 **MP (°C):**

MW: 805.98 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.400E-04	5.964E-01	ns	B425	0 0 0 1 0	

4590. C₄₂H₆₂N₈O₇

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[3-(aminomethyl)phenyl]methyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-

RN: 100901-98-2 **MP (°C):**

MW: 791.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.400E-03	1.107E+00	ns	B425	0 0 0 1 0	pH 7.4

4591. C₄₂H₇₀O₃₅

β-Cyclodextrin

β-Cyclodextrin hydrate

Cycloheptaamyllose hydrate

Cyclodextrin hydrate

RN: 7585-39-9 **MP (°C):** 298–300

MW: 1135.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.044E-02	1.185E+01	15	W317	2 2 1 0 2	
1.216E-02	1.381E+01	20	F186	1 2 1 1 1	
1.282E-02	1.455E+01	20	W317	2 2 1 0 2	
1.410E-02	1.600E+01	21	C407	1 0 1 2 1	
1.540E-02	1.748E+01	23.7	J305	0 0 0 0 0	
1.630E-02	1.850E+01	25	B396	0 0 0 0 0	
1.586E-02	1.800E+01	25	C407	1 0 1 2 1	
1.558E-02	1.768E+01	25	H319	0 0 0 0 0	
1.600E-02	1.816E+01	25	O304	1 2 2 2 2	
1.600E-02	1.816E+01	25	O321	0 0 0 0 0	
1.621E-02	1.840E+01	25	S462	0 0 0 0 0	
1.674E-02	1.900E+01	25	T425	0 0 0 0 0	
1.551E-02	1.760E+01	25	W317	2 2 1 0 2	
1.630E-02	1.850E+01	25.0	J305	0 0 0 0 0	
2.026E-02	2.300E+01	30	C407	1 0 1 2 1	
1.895E-02	2.151E+01	30	W317	2 2 1 0 2	
2.203E-02	2.500E+01	35	C407	1 0 1 2 1	
2.440E-02	2.769E+01	35.0	J305	0 0 0 0 0	
3.100E-02	3.519E+01	40	O321	0 0 0 0 0	
2.980E-02	3.382E+01	40.0	J305	0 0 0 0 0	

(continued)

4591. C₄₂H₇₀O₃₅ (continued)

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.850E-02	4.370E+01	45.0	J305	0 0 0 0 0	
4.430E-02	5.028E+01	48.0	J305	0 0 0 0 0	
4.400E-02	4.994E+01	55	O321	0 0 0 0 0	
1.558E-02	1.768E+01	ns	M335	0 0 2 0 1	

4592. C₄₂H₇₀O₃₅6-O- α -D-Glucosyl- α -cyclodextrin

RN: MP (°C):

MW: 1135.01 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.000E-01	9.080E+02	25	O321	0 0 0 0 0	
1.030E+00	1.169E+03	40	O321	0 0 0 0 0	
1.190E+00	1.351E+03	55	O321	0 0 0 0 0	

4593. C₄₃H₅₅NO₁₃

Docetaxel

Taxotere

N-Debenzoyl-*N*-*tert*-butoxycarbonyl-10-deacetyl taxol

RN: 114977-28-5 MP (°C):

MW: 793.92 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.557E-06	6.000E-03	22.5	C438	0 0 0 0 0	

4594. C₄₃H₅₈N₄O₁₂

Rifampin

Rifampicin

RN: 13292-46-1 MP (°C):

MW: 822.96 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.300E-01	1.070E+02	25	B073	2 1 2 2 2	pH 2.12, <i>sic</i>
4.374E-03	3.600E+00	25	B073	2 1 2 2 1	pH 2.5
1.701E-03	1.400E+00	25	B073	2 1 2 2 1	pH 5.33
1.215E-03	1.000E+00	25	B073	2 1 2 2 1	pH 3.99
1.215E-03	1.000E+00	25	B073	2 1 2 2 1	pH 3.03
1.580E-03	1.300E+00	25	G096	1 0 0 0 0	pH 4.3
1.215E-04	1.000E-01	ns	K444	0 0 0 0 0	
3.393E-03	2.792E+00	rt	F182	0 0 0 0 1	pH 7.5

4595. C₄₃H₆₁N₇O₁₀

L-Histidinamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-*N*-[4-[[1-[[[[3-(carboxymethoxy)phenyl]methyl]amino]carbonyl]-3-methylbutyl]amino]-2-hydroxy-1-(2-methylpropyl)-4-oxobutyl]-, [1*S*-[1*R**,2*R**,4(*R**)]]-

RN: 100902-05-4 **MP (°C):**

MW: 836.01 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.700E-04	2.257E-01	ns	B425	0 0 0 1 0	

4596. C₄₃H₆₂N₈O₇

L-threo-Pentonamide, 5-cyclohexyl-2,4,5-trideoxy-4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-*N*-[3-methyl-1-[(4-pyridinylmethyl)amino]carbonyl]butyl]-

RN: 105192-86-7 **MP (°C):**

MW: 803.02 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<8.03E-03	ns	B425	0 0 0 1 0	pH 7.4

4597. C₄₃H₆₂N₈O₈

L-Phenylalaninamide, *N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-L-histidyl-(3*S*,4*S*)-4-amino-3-hydroxy-6-methylheptanoyl-L-leucyl-

L-Phenylalaninamide, *N*-[4-[[*N*-[*N*-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl-,

RN: **MP (°C):**

MW: 819.02 **BP (°C):** 1171.2

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<2.00E-05	<1.64E-02	ns	B425	0 0 0 1 0	pH 7.4

4598. C₄₃H₇₅NO₁₆

Erythromycin ethyl succinate

RN: 1264-62-6 **MP (°C):**

MW: 862.07 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.262E-04	1.950E-01	21	M044	2 0 2 2 2	

4599. C₄₄H₅₆O₄*p-tert-Butylcalix[4]arenenetetrol*Tetra-*p-tert-butyltetralcalix[4]arene**p-tert-Butylcalix[4]arene**p-tert-Butylcalix[4]arene-25,26,27,28-tetrol*Formaldehyde-*p-tert-butylphenyl* cyclic tetramer5,11,17,23-Tetra-*p-tert-butyl-25,26,27,28-tetrahydroxycalix(4)arene***RN:** 60705-62-6 **MP (°C):** 342-346**MW:** 648.93 **BP (°C):** 683.1

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<6.49E-03	25	B424	1 0 1 2 2	

4600. C₄₄H₆₄N₈O₉

D-Phenylalanine, 3-(aminomethyl)-N-[N-[4-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-3-hydroxy-6-methyl-1-oxoheptyl]-L-leucyl]-

RN: 115511-03-0 **MP (°C):****MW:** 849.05 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.900E-04	3.311E-01	ns	B425	0 0 0 1 0	pH 7.4

4601. C₄₄H₆₉NO₁₀

Tacrolimus

FK506

RN: 104987-11-3 **MP (°C):****MW:** 772.04 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.580E-06	1.220E-03	25	A410	1 0 2 2 1	

4602. C₄₄H₇₄O₃₄*n-Ethyl-paba-β-cyclodextrin***RN:** **MP (°C):****MW:** 1147.06 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.100E-03	5.850E+00	ns	F327	0 0 1 2 2	

4603. C₄₄H₇₄O₃₅Hydroxyethyl- β -cyclodextrin

RN: MP (°C):
MW: 1163.06 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.224E-01	3.750E+02	ns	M335	0 0 2 0 1	

4604. C₄₅H₆₃Cl₂NO₆

Cosalane

RN: 154212-56-3 MP (°C): 262 C
MW: 784.91 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.784E-09	1.400E-06	ns	V417	0 0 0 0 0	

4605. C₄₅H₆₆N₈O₇

L-Histidinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl-N-[2-hydroxy-4-[[3-methyl-1-[[4-(phenylmethyl)-1-piperazinyl]carbonyl]butyl]amino]-1-(2-methylpropyl)-4-oxobutyl]-

RN: 105192-85-6 MP (°C):
MW: 831.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<8.31E-03	ns	B425	0 0 0 1 0	pH 7.4

4606. C₄₅H₆₆N₈O₇

L-threo-Pentonamide, N-[1-[[[3-(aminomethyl)phenyl]methyl]amino]carbonyl]-3-methylbutyl]-5-cyclohexyl-2,4,5-trideoxy-4-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-

RN: 100902-07-6 MP (°C):
MW: 831.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.000E-05	1.662E-02	ns	B425	0 0 0 1 0	pH 7.4

4607. C₄₅H₇₃NO₁₅

Solanine

β -D-Galactopyranoside, (3 β)-solanid-5-en-3-yl O-6-deoxy- α -L-mannopyranosyl-(1 \otimes 2)-O-[β -D-glucopyranosyl-(1-3)]-

Solanidine, β -D-galactopyranoside deriv

RN: 20562-02-1 MP (°C):

MW: 868.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	2.604E-02	15	K059	2 2 2 0 0	

4608. C₄₅H₇₆O₃₅*n*-Propyl-paba- β -cyclodextrin

RN: MP (°C):

MW: 1177.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.100E-03	2.472E+00	ns	F327	0 0 1 2 2	

4609. C₄₆H₆₂N₄O₁₁

Rifabutin

1',4-Didehydro-1-deoxy-1,4-dihydro-5'-(2-methylpropyl)-1-oxo

Ansamycin

Antibiotic LM 427

LM 427

Mycobutin

RN: 72559-06-9 MP (°C):

MW: 847.03 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.243E-04	1.900E-01	ns	S469	0 0 0 0 0	

4610. C₄₆H₆₅N₇O₁₀

Acetic acid, [3-[[[2-[[5-cyclohexyl-2,4,5-trideoxy-4-[[N-[N-[(1,1-dimethylethoxy)carbonyl]-L-phenylalanyl]-L-histidyl]amino]-L-threo-pentonoyl]amino]-4-methyl-1-oxopentyl]amino]methyl]phenoxy]-

RN: 100902-09-8 MP (°C):

MW: 876.07 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-05	2.628E-02	ns	B425	0 0 0 1 0	

4611. C₄₆H₇₇NO₁₇

Tylosin

Vubityl 200

Vetil(R)

RN: 1401-69-0 MP (°C): 128

MW: 916.12 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.195E-03	7.508E+00	21	M044	2 0 2 2 2	

4612. C₄₆H₇₈O₃₅

n-Butyl-paba-β-cyclodextrin

RN: MP (°C):

MW: 1191.11 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	8.338E-01	ns	F327	0 0 1 2 2	

4613. C₄₇H₅₁NO₁₄

Paclitaxel

5-β,20-Epoxy-1,2-α,4,7-β,10-β,13-α-hexahydroxy-tax-11-en-9-one 4,10-diacetate 2-benzoate 13-ester with (2*R*,3*S*)-*N*-benzoyl-3-phenyl-isoserine

TAX

Taxal

Taxol

Taxol A

RN: 33069-62-4 MP (°C): 213–216

MW: 853.93 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.513E-07	3.000E-04	37	L435	0 0 0 0 0	
1.569E-06	1.340E-03	37	V412	0 0 0 0 0	

4614. C₄₇H₇₃NO₁₇

Amphotericin B

RN: 1397-89-3 MP (°C):

MW: 924.10 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.116E-04	7.500E-01	28	A038	2 0 1 1 1	
3.246E-06	3.000E-03	ns	K067	0 0 2 1 0	intrinsic

4615. C₄₇H₇₅NO₁₇

Nystatin

Mycostatin

Biofanal

Nystex

Fungicidin

RN: 1400-61-9

MP (°C):

MW: 926.12

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.887E-04	3.600E-01	24	M166	2 0 0 1	
4.319E-03	4.000E+00	ns	K444	0 0 0 0	

4616. C₄₈H₇₂O₁₄

Ivermectin

Heartgard-30

Ivomec

RN: 70288-86-7

MP (°C):

MW: 873.10

BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.581E-06	4.000E-03	ns	K444	0 0 0 0	

4617. C₄₈H₈₀O₄₀

6-O-α-D-Maltosyl-α-cyclodextrin

6-O-α-Maltosyl-α-cyclodextrin

RN: MP (°C):

MW: 1297.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.700E-01	9.988E+02	25	O321	0 0 0 0	
2.400E-01	3.113E+02	25	O321	0 0 0 0	
7.700E-01	9.988E+02	40	O321	0 0 0 0	
3.500E-01	4.540E+02	40	O321	0 0 0 0	
1.330E+00	1.725E+03	55	O321	0 0 0 0	
5.400E-01	7.005E+02	55	O321	0 0 0 0	

4618. C₄₈H₈₀O₄₀

γ -Cyclodextrin
Cyclooctaamyllose
Ringdex C
Cyclomaltooctaoose
Dexy Pearl γ -100

RN: 17465-86-0 **MP (°C):**

MW: 1297.15 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.338E-01	1.736E+02	20	F186	1 2 1 1 1	
1.789E-01	2.320E+02	25	B396	0 0 0 0 0	
2.000E-01	2.594E+02	25	O321	0 0 0 0 0	
1.921E-01	2.492E+02	25	S462	0 0 0 0 0	
1.680E-01	2.179E+02	25.0	J305	0 0 0 0 0	
2.040E-01	2.646E+02	30.0	J305	0 0 0 0 0	
2.430E-01	3.152E+02	35.0	J305	0 0 0 0 0	
4.300E-01	5.578E+02	40	O321	0 0 0 0 0	
2.680E-01	3.476E+02	40.0	J305	0 0 0 0 0	
3.110E-01	4.034E+02	42.0	J305	0 0 0 0 0	
6.400E-01	8.302E+02	55	O321	0 0 0 0 0	
1.452E-01	1.883E+02	ns	M335	0 0 2 0 1	

4619. C₄₉H₈₇NS

Erythromycin lactobionate

RN: 3847-29-8 **MP (°C):** 145

MW: 722.31 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>2.77E-02	>2.00E+01	21	M044	2 0 2 2 0	

4620. C₅₀H₈₂N₁₀O₃₁S₁₀

Decane(*S*-(carboxymethyl)-L-cysteine))

RN: **MP (°C):**

MW: 1639.90 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.820E-05	9.544E-02	15	N331	0 0 0 0 0	
5.730E-04	9.397E-01	25	N331	0 0 0 0 0	

4621. C₅₁H₅₅NO₁₈

7-Malyl paclitaxel

RN: 265659-44-7 MP (°C): 166–168

MW: 970.00 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.093E-04	3.000E-01	ns	D401	0 2 2 2 0	

4622. C₅₁H₅₅NO₁₈

2'-Malyl paclitaxel

RN: 265659-38-9 MP (°C): 148–151

MW: 970.00 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.062E-04	2.000E-01	ns	D401	0 2 2 2 0	

4623. C₅₁H₇₀N₁₂O₁₁

His-pro-D-phe-his-leu-leu-thr-tyr

RN: MP (°C):

MW: 1027.20 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.100E-05	8.320E-02	20	B141	1 2 0 0 1	pH 7.5

4624. C₅₁H₇₄O₁₉

Penta-acetyl-gitoxin

RN: 7242-04-8 MP (°C):

MW: 991.15 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.200E-05	1.189E-02	ns	M070	0 0 0 0 1	

4625. C₅₂H₇₂N₁₂O₁₀

His-pro-phe-his-leu-leu-val-tyr

RN: MP (°C):

MW: 1025.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.610E-04	1.651E-01	ns	B141	0 2 0 0 2	pH 7.5

4626. C₅₂H₇₂N₁₂O₁₀

His-pro-phe-his-leu-d-leu-val-tyr

RN: MP (°C):

MW: 1025.23 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.370E-04	1.405E-01	ns	B141	0 2 0 0 2	pH 7.5

4627. C₅₂H₈₈O₃₉*n*-Butyl-paba- γ -cyclodextrin

RN: MP (°C):

MW: 1337.26 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
7.000E-04	9.361E-01	ns	F327	0 0 1 2 2	

4628. C₅₂H₉₇NO₁₈S

Erythromycin estolate

RN: 3521-62-8 MP (°C): 135

MW: 1056.41 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.515E-04	1.600E-01	21	M044	2 0 2 2 2	

4629. C₅₄H₉₀O₄₅6-*O*- α -D-Glucosyl- γ -cyclodextrin

RN: MP (°C):

MW: 1459.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.800E-01	1.430E+03	25	O321	0 0 0 0 0	
1.010E+00	1.474E+03	40	O321	0 0 0 0 0	
1.180E+00	1.722E+03	55	O321	0 0 0 0 0	

4630. C₅₄H₉₀O₄₅6-*O*- α -D-Maltosyl- β -cyclodextrin6-*O*- α -Maltosyl- β -cyclodextrin

RN: MP (°C):

MW: 1459.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.040E+00	1.518E+03	25	O321	0 0 0 0 0	
1.040E+00	1.518E+03	40	O321	0 0 0 0 0	
1.220E+00	1.780E+03	55	O321	0 0 0 0 0	

4631. C₅₄H₉₀O₄₅

6-O- α -D-Maltotriosyl- α -cyclodextrin
6-O- α -Maltotriosyl- α -cyclodextrin

RN: MP (°C):
MW: 1459.29 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.070E+00	1.561E+03	25	O321	0 0 0 0 0	
1.220E+00	1.780E+03	40	O321	0 0 0 0 0	
1.370E+00	1.999E+03	55	O321	0 0 0 0 0	

4632. C₅₅H₅₉NO₂₂

2',7'-bis-(Mallyl) paclitaxel

RN: 265659-41-4 MP (°C): 166–168
MW: 1086.08 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.604E-04	5.000E-01	ns	D401	0 2 2 2 0	

4633. C₅₅H₇₀N₁₂O₁₀

His-pro-phe-his-leu-phe-val-tyr

RN: MP (°C):
MW: 1059.25 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.760E-04	1.864E-01	ns	B141	0 2 0 0 2	pH 7.5

4634. C₅₅H₇₉N₁₃O₁₁

His-pro-D-phe-his-leu-leu-val-tyr-serinol

RN: MP (°C):
MW: 1098.32 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.000E-04	3.295E-01	20	B141	1 2 0 0 2	pH 7.5

4635. C₅₅H₉₀N₁₁O₃₄S₁₁

Undecane(*S*-(carboxymethyl)-L-cysteine))

RN: MP (°C):
MW: 1802.09 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.200E-06	1.658E-02	15	N331	0 0 0 0 0	
1.340E-04	2.415E-01	25	N331	0 0 0 0 0	
2.900E-04	5.226E-01	35	N331	0 0 0 0 0	

4636. C₅₆H₉₈O₃₅

β -Cyclodextrin, tetradeca-*O*-methyl-
Heptakis(2,6-di-*O*-methyl)- β -cyclodextrin

RN: 188367-19-3 MP (°C):
MW: 1331.38 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.727E-01	3.631E+02	25	H319	0 0 0 0 0	

4637. C₅₇H₇₉N₁₃O₁₁

Pro-his-pro-phe-his-leu-leu-val-tyr
RN: MP (°C):
MW: 1122.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.240E-04	3.636E-01	ns	B141	0 2 0 0 2	pH 7.5

4638. C₅₇H₇₉N₁₃O₁₁

Pro-his-pro-phe-his-leu-D-leu-val-tyr
RN: MP (°C):
MW: 1122.35 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
4.100E-05	4.602E-02	ns	B141	0 2 0 0 1	pH 7.5

4639. C₆₀H₇₇N₁₃O₁₁

Pro-his-pro-phe-his-leu-phe-val-tyr
RN: MP (°C):
MW: 1156.36 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.430E-04	3.966E-01	ns	B141	0 2 0 0 2	pH 7.5

4640. C₆₀H₉₂N₁₂O₁₀

Gramicidin S
Gramicidin
Cyclo(L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl-L-leucyl-D-phenylalanyl-L-prolyl-L-valyl-L-ornithyl)
Gramicidin S-A

RN: 113-73-5 MP (°C):
MW: 1141.48 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.226E-04	1.400E-01	28	A038	2 0 1 1 2	

4641. C₆₀H₉₈N₁₂O₃₇S₁₂Dodecane(*S*-(carboxymethyl)-L-cystein))

RN: MP (°C):

MW: 1964.28 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.300E-06	4.518E-03	15	N331	0 0 0 0 0	
2.400E-05	4.714E-02	25	N331	0 0 0 0 0	
5.880E-05	1.155E-01	35	N331	0 0 0 0 0	

4642. C₆₀H₁₀₀O₅₀6-*O*-α-D-Maltotriosyl-β-cyclodextrin6-*O*-α-Maltotriosyl-β-cyclodextrin6-*O*-α-D-Maltosyl-γ-cyclodextrin6-*O*-α-Maltosyl-γ-cyclodextrin

RN: MP (°C):

MW: 1621.44 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.400E-01	1.524E+03	25	O321	0 0 0 0 0	
9.400E-01	1.524E+03	40	O321	0 0 0 0 0	
1.140E+00	1.848E+03	55	O321	0 0 0 0 0	
1.100E+00	1.784E+03	55	O321	0 0 0 0 0	

4643. C₆₂H₈₆N₁₂O₁₆

Actinomycin D

Actactinomycin A IV

Actinomycin AIV

Actinomycin I1

RN: 50-76-0 MP (°C):

MW: 1255.45 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.983E-04	5.000E-01	37	G025	1 0 0 0 1	
7.965E-04	1.000E+00	rt	G025	0 0 0 0 1	

4644. C₆₂H₁₁₁N₁₁O₁₂

Cyclosporin A

1,4,7,10,13,16,19,22,25,28,31-Undecaazacyclotri(triacontane, cyclic peptide deriv.

Sandimmun neoral

Sandimmun

Sang-35

SDZ-OXL 400

RN: 59865-13-3 MP (°C): 148–151

MW: 1202.64 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.326E-05	4.000E-02	25	B376	0 0 0 0 0	
8.315E-06	1.000E-02	amb	L434	0 0 0 0 0	

4645. C₆₃H₈₅N₂₁O₁₉

Candididin

Candeptin

Vanobid

RN: 1403-17-4 MP (°C):

MW: 1440.51 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.349E-03	1.347E+01	21	M044	2 0 2 2 2	

4646. C₆₃H₈₈N₁₄O₁₄PCo

Vitamin B12

Cyanoject

Hydrobexan

Alphamine

Crystamine

Cyomin

RN: 68-19-9 MP (°C):

MW: 1355.40 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
9.149E-03	1.240E+01	20	F300	1 0 0 0 2	

4647. C₆₄H₁₁₂O₄₀Dimethyl- β -cyclodextrin β -Cyclodextrin, 2A,2B,2C,2D,2E,2F,2G,6A,6B,6C,6D,6E,6F,6G-Tetradeca-*O*-methyl-Heptakis(2,6-di-*O*-methyl)- β -cyclodextrinTetradeca-*O*-methyl- β -cyclodextrinTetradecakis-2,6-*O*-methylcycloheptaamyllose

RN: 51166-71-3 MP (°C): 298–300

MW: 1521.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.397E-01	2.126E+02	c	D316	0 0 0 0 0	

4648. C₆₅H₁₀₆N₁₃O₄₀S₁₃Tridecane(*S*-(carboxymethyl)-L-cysteine))

RN: MP (°C):

MW: 2126.46 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-06	1.318E-02	25	N331	0 0 0 0 0	
1.600E-05	3.402E-02	35	N331	0 0 0 0 0	

4649. C₆₆H₈₄O₆4-*tert*-Butylcalix[6]arene5,11,17,23,29,35-Hexa-*tert*-butyl-37,38,39,40,41,42-hexahydroxycalix[6]arene

RN: 78092-53-2 MP (°C): 380–381

MW: 973.40 BP (°C): 890.5

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
<1.00E-05	<9.73E-03	25	B424	1 0 1 2 2	

4650. C₆₆H₁₁₀O₅₅6-*O*- α -D-Maltotriosyl- γ -cyclodextrin6-*O*- α -Maltotriosyl- γ -cyclodextrin

RN: MP (°C):

MW: 1783.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.500E-01	1.516E+03	25	O321	0 0 0 0 0	
8.500E-01	1.516E+03	40	O321	0 0 0 0 0	
1.040E+00	1.855E+03	55	O321	0 0 0 0 0	

4651. C₆₇H₉₃N₁₅O₁₃

Pro-pro-pro-his-pro-phe-his-leu-d-leu-val-tyr

RN: MP (°C):

MW: 1316.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.650E-04	4.806E-01	ns	B141	0 2 0 0 2	pH 7.5

4652. C₆₇H₉₃N₁₅O₁₃

Pro-pro-pro-his-pro-phe-his-leu-leu-val-tyr

RN: MP (°C):

MW: 1316.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.750E-04	4.937E-01	ns	B141	0 2 0 0 2	pH 7.5

4653. C₇₀H₈₉N₁₅O₁₃

Pro-pro-pro-his-pro-phe-his-leu-phe-val-tyr

RN: MP (°C):

MW: 1348.58 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
2.240E-04	3.021E-01	ns	B141	0 2 0 0 2	pH 7.5

4654. C₇₀H₁₂₆O₃₅β-Cyclodextrin, tetradeca-*O*-ethyl-Heptakis(2,6-di-*O*-ethyl)-β-cyclodextrin

RN: 194715-43-0 MP (°C):

MW: 1527.76 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.273E-05	5.000E-02	25	H319	0 0 0 0 0	

4655. C₇₂H₈₅N₁₉O₁₈S₅

Thiostrepton

Bryamycin

RN: 1393-48-2 MP (°C): 210

MW: 1664.92 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
5.286E-05	8.800E-02	21	M044	2 0 2 2 1	
1.442E-04	2.400E-01	28	A038	2 0 1 1 1	

4656. C₇₂H₁₀₀N₁₈O₁₇PCo

Coenzyme B12

Cobamamide

Cobalamin, Co-(5'-deoxy-5'-adenosyl)-

Dibencozide

Funacomide

Deoxyadenosylcobalamin

RN: 13870-90-1 **MP (°C):****MW:** 1579.62 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.646E-02	2.600E+01	24	M054	1 0 0 0 1	

4657. C₇₄H₁₀₀ClN₁₅O₁₄

Antarelix

AcdNal-Dcpa-ser-tyr-dhai-leu-lys(ipr)-pro-dala-NH2

RN: 151272-78-5 **MP (°C):****MW:** 1459.17 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
>6.85E-03	>1.00E+01	ns	D350	0 1 0 1 1	

4658. C₇₅H₁₂₂N₁₅O₄₆S₁₅

Pendecane(S-(carboxymethyl)-L-cysteine))

RN: **MP (°C):****MW:** 2450.84 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
3.400E-07	8.333E-04	25	N331	0 0 0 0 0	

4659. C₇₇H₁₀₇N₁₇O₁₅

Pro-pro-pro-pro-his-pro-phe-his-leu-leu-val-tyr

RN: **MP (°C):****MW:** 1510.82 **BP (°C):**

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
1.328E-03	2.006E+00	ns	B141	0 2 0 0 2	pH 7.5

4660. C₈₀H₁₀₅N₁₇O₁₅

Pro-pro-pro-pro-his-pro-phe-his-leu-phe-val-tyr

RN: MP (°C):

MW: 1544.83 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
8.400E-04	1.298E+00	ns	B141	0 2 0 0 2	pH 7.5

4661. C₈₅H₁₁₇N₂₀O₁₈

Asp-arg-val-tyr-ile-his-pro-d-phe-his-leu-phe-val-tyr

RN: MP (°C):

MW: 1707.00 BP (°C):

Solubility (Moles/L)	Solubility (Grams/L)	Temp (°C)	Ref (#)	Evaluation (T P E A A)	Comments
6.200E-05	1.058E-01	20	B141	1 2 0 0 1	pH 7.5

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