Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Electronic Supplementary Information

Classification of baseline toxicants for QSAR predictions to replace fish acute toxicity studies

Monika Nendza[1]*, Martin Müller[2] and Andrea Wenzel[2]
[1] Analytical Laboratory AL-Luhnstedt, Bahnhofstraße 1, 24816 Luhnstedt, Germany
[2] Fraunhofer Institute for Molecular Biology and Applied Ecology IME, Auf dem Aberg 1, 57392 Schmallenberg, Germany

S1. Additional information on the training set

Fish acute toxicity data for *Pimephales promelas* were taken from the EPA Fathead Minnow acute toxicity database (EPAFHM).[1] The EPAFHM contains high quality data, obtained consistently with the same fish species in the same laboratory. Exclusion of inorganic compounds (n=1), organometallic compounds (n=3), organic salts and complexes (n=22), and compounds without an LC_{50} value (n=36) resulted in a dataset of 96h LC_{50} data [mmol/L] for 555 discrete organic compounds (447 baseline, 108 excess) with a range in molecular weight from 32.0 to 488.6 g/mol and calculated[2] log K_{ow} from -4.15 to 7.43 (Table S1).

Chemicals were grouped as either baseline or excess toxicants based on their experimental fish acute toxicity data relative to a log K_{ow}-dependent baseline QSAR[3] for acute fish toxicities [96-h LC_{50} (*Pimephales promelas*): log $1/LC_{50}$ [mmol/L] = 0.79 log K_{ow} - 1.35, where n = 147, r = 0.92, s = 0.40; n is the number of observations, r is the correlation coefficient and s is the standard deviation of the residuals]. The toxicity estimates were compared to the available experimental fish acute toxicity data. If calculated and experimental toxicity data agreed within a factor of 10, i.e. residuals (log $1/LC_{50\ exp}$ - log $1/LC_{50\ calc}$) <1 log unit, chemicals were considered baseline toxicants. Excess toxicity as introduced by Lipnick[4, 5] refers to enhanced effects of compounds relative to their baseline toxicity. Excess toxicity significantly, at least 10-times, exceeds the calculated baseline toxicity. Deviations larger than a factor of 10, i.e. residuals (log $1/LC_{50\ exp}$ - log $1/LC_{50\ calc}$) >1 log unit, prompted assignment of excess toxicity. Note that excess toxicities are based on a formal comparison of the experimental and calculated numeric values and may be due to diverse MOA related to the chemical reactivities of the toxicants with biological targets.[6]

Table S1: Training set of fish acute toxicity data.

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals (log $1/LC_{50exp}$ - log $1/LC_{50calc}$)
100-01-6	p-Nitroaniline	1.47	125	0.23
100-02-7	p-Nitrophenol	1.91	44.8	0.33
100-10-7	p-Dimethylaminobenzaldehyde	1.89	45.7	0.37
100-25-4	1,4-Dinitrobenzene	1.63	0.709	2.44
10031-82-0	p-Ethoxybenzaldehyde	2.28	28.1	0.28
100-37-8	N,N-Diethylethanolamine	0.05	1780	0.13
100-41-4	Ethylbenzene	3.03	10.5	-0.04
100-46-9	Benzylamine	1.07	102	0.53
100-52-7	Benzaldehyde	1.71	9.87	1.03
100-61-8	N-Methylaniline	1.62	100	0.10
100-64-1	Cyclohexanone oxime	0.91	208	0.37
100-70-9	2-Cyanopyridine	0.35	726	0.23
100-71-0	2-Ethylpyridine	1.84	414	-0.69
100-79-8	Solketal	1.07	16700	-1.60
100-97-0	Hexamethylenetetramine (aliphatic)	-4.15	49800	2.08
101-84-8	Phenyl ether	4.05	4	-0.22
102-27-2	N-Ethyl-m-toluidine	2.66	49.5	-0.31
102-69-2	Tripropylamine	2.99	50.9	-0.56
102-71-6	Triethanolamine	-2.48	11800	1.41
10293-06-8	[1(R)-endo]-(+)-3-Bromocamphor	3.31	68.4	-0.74
103-05-9	Benzyl-tert-butanol	2.93	66.4	-0.57
103-76-4	1-(2-Hydroxyethyl)piperazine	-1.56	6410	0.89
103-83-3	N,N-Dimethylbenzylamine	1.75	37.9	0.52
103-90-2	4-Acetamidophenol	0.27	814	0.41
104-13-2	4-Butylaniline	3.10	10.1	0.07
10453-86-8	Resmethrin	7.11	0.00616	0.47
104-76-7	2-Ethyl-1-hexanol	2.73	28.3	-0.14
104-88-1	4-Chlorobenzaldehyde	2.35	2.19	1.30
104-90-5	5-Ethyl-2-methylpyridine	2.39	81.1	-0.36

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
105-14-6	5-Diethylamino-2-pentanone	0.94	336	0.28
105-53-3	Diethyl malonate	0.90	14.7	1.68
105-67-9	2,4-Dimethylphenol	2.61	16.6	0.15
105-75-9	Dibutyl fumarate	4.16	0.63	0.62
105-99-7	Dibutyl adipate	4.33	3.64	-0.22
106-40-1	p-Bromoaniline	1.97	47.5	0.35
106-42-3	p-Xylene	3.09	8.86	-0.01
106-44-5	4-Methylphenol (p-cresol)	2.06	16.5	0.54
106-47-8	4-Chloroaniline	1.72	31.4	0.60
106-48-9	4-Chlorophenol	2.16	6.11	0.97
106-49-0	4-Toluidine	1.62	160	-0.10
106-63-8	Isobutyl acrylate	2.13	2.1	1.45
106-94-5	1-Bromopropane	2.16	67.3	-0.09
107-02-8	Acrolein	0.19	0.017	4.72
107-06-2	1,2-Dichloroethane	1.83	136	-0.23
107-07-3	2-Chloroethanol	0.11	53.7	1.44
107-10-8	Propylamine	0.34	308	0.36
107-12-0	Propionitrile	0.35	1520	-0.37
107-14-2	Chloroacetonitrile	0.11	1.34	3.01
107-15-3	Ethylenediamine	-1.62	220	2.07
107-18-6	Allyl alcohol	0.21	0.32	3.44
107-19-7	2-Propyn-1-ol	-0.42	1.48	3.26
1072-97-5	2-Amino-5-bromopyridine	1.42	177	0.22
107-29-9	Acetaldoxime	-0.21	76	1.41
107-41-5	2-Methyl-2,4-pentanediol	0.58	10700	-1.07
107-45-9	tert-Octylamine	2.58	24.6	0.03
107-47-1	tert-Butyl sulfide	3.64	29.1	-0.82
107-87-9	2-Pentanone	0.75	1240	-0.40
1080-32-6	Diethyl benzylphosphonate	1.56	336	-0.05
108-10-1	4-Methyl-2-pentanone	1.16	522	-0.28
108-20-3	Isopropyl ether	1.88	786	-1.02
108-88-3	Toluene	2.54	33.9	-0.22
108-89-4	4-Picoline	1.35	403	-0.35
108-90-7	Chlorobenzene	2.64	16.9	0.09
108-93-0	Cyclohexanol	1.64	704	-0.79
108-94-1	Cyclohexanone	1.13	621	-0.34
108-95-2	Phenol	1.51	32.7	0.62
108-99-6	3-Picoline	1.35	144	0.09
109-01-3	1-Methylpiperazine	-0.59	2300	0.46
109-06-8	2-Picoline	1.35	897	-0.70
109-07-9	2-Methylpiperazine	-0.38	2240	0.30
109-60-4	Propyl acetate	1.36	60	0.51
109-64-8	1,3-Dibromopropane	2.50	2.1	1.36
109-65-9	1-Bromobutane	2.65	36.7	-0.17
109-73-9	Butylamine	0.83	268	0.13
109-75-1	Allyl cyanide	0.70	182	0.36
109-76-2	1,3-Diaminopropane	-1.13	1190	1.04
109-77-3	Malononitrile	-0.60	0.56	3.90
109-85-3	2-Methoxyethylamine	-0.91	524	1.23
109-89-7	Diethylamine	0.81	855	-0.36
109-97-7	Pyrrole	0.88	210	0.16
109-99-9	Tetrahydrofuran	0.94	2160	-0.87
110-00-9	Furan	1.36	61	0.32
110-06-5	t-Butyl disulfide	4.60	1.37	-0.17
110-12-3	5-Methyl-2-hexanone	1.66	159	-0.11
110-40-7	Diethyl sebacate	4.33	2.71	-0.09
110-43-0	2-Heptanone	1.73	131	-0.08
110-54-3	Hexane	3.29	2.5	0.29
110-56-5	1,4-Dichlorobutane	2.81	51.6	-0.48
110-58-7	Amylamine	1.33	177	-0.01
110-62-3	Valeraldehyde	1.31	12.9	1.14
110-65-6	2-Butyne-1,4-diol	-0.93	53.6	2.29
110-73-6	2-(Ethylamino)ethanol	-0.66	1480	0.65

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
110-82-7	Cyclohexane	3.18	4.53	0.11
110-86-1	Pyridine	0.80	99.8	0.62
110-88-3	s-Trioxane	-0.56	5950	-0.03
110-93-0	6-Methyl-5-hepten-2-one	2.06	85.7	-0.11
111-13-7	2-Octanone	2.22	36	0.15
111-15-9	2-Ethoxyethyl acetate	0.59	42.2	1.38
111-25-1	1-Bromohexane	3.63	3.45	0.16
111-26-2	Hexylamine	1.82	56.6	0.16
111-27-3	1-Hexanol	1.82	97.7	-0.07
111-42-2	Diethanolamine	-1.71	4710	1.05
111-46-6	2-Hydroxyethyl ether	-1.47	75200	-0.34
111-47-7	n-Propyl sulfide	2.88	21.8	-0.19
111-68-2	n-Heptylamine	2.31	21.8	0.25
111-69-3	1,4-Dicyanobutane	0.35	1930	-0.18
111-70-6	1-Heptanol	2.31	34.5	0.05
111-83-1	1-Bromooctane	4.61	0.838	0.07
111-86-4	Octylamine	2.80	5.2	0.53
111-87-5	1-Octanol	2.81	13.5	0.11
111-90-0	2-(2-Ethoxyethoxy)ethanol	-0.69	26500	-0.40
112-05-0	Nonanoic acid	3.52	104	-1.25
112-12-9	2-Undecanone	3.69	1.5	0.49
112-20-9	Nonylamine	3.29	2.15	0.57
1122-54-9	4-Acetyl pyridine	0.49	168	0.82
112-27-6	Triethylene glycol	-1.75	68900	0.07
112-30-1	1-Decanol	3.79	2.41	0.17
1126-46-1	Methyl p-chlorobenzoate	2.47	10.9	0.59
1126-79-0	Butyl phenyl ether	3.55	5.71	-0.03
1129-35-7	Methyl 4-cyanobenzoate	1.38	46.7	0.80
114-26-1	Propoxur (Baygon)	1.90	8.81	1.22
115-19-5	2-Methyl-3-butyn-2-ol	0.45	3290	-0.60
115-20-8	2,2,2-Trichloroethanol	1.21	299	0.09
115-32-2	Dicofol (Kelthane)	5.81	0.619	-0.46
115-86-6	Triphenyl phosphate	4.70	0.868	0.21
115-90-2	Fensulfothion	2.35	43.2	0.35
116-06-3	Aldicarb	1.36	0.86	2.62
118-55-8	Phenyl salicylate	3.82	1.18	0.59
118-61-6	Ethyl salicylate	3.09	20.3	-0.18
118-79-6	2,4,6-Tribromophenol	4.18	6.55	-0.25
119-34-6	4-Amino-2-nitrophenol	0.64	36.2	1.47
119-61-9	Benzophenone	3.15	14.7	-0.05
1198-55-6	Tetrachlorocatechol	3.61	1.27	0.79
120-07-0	N-Phenyldiethanolamine	0.63	735	0.24
120-21-8	4-(Diethylamino)benzaldehyde	2.87	23.9	-0.05
1204-21-3	alpha-Bromo-2',5'-dimethoxyacetophenone	2.18	0.661	2.22
120-80-9	Catechol	1.03	9.22	1.61
120-82-1	1,2,4-Trichlorobenzene	3.93	2.99	0.03
120-83-2	2,4-Dichlorophenol	2.80	7.74	0.46
121-14-2	2,4-Dinitrotoluene	2.18	24.2	0.50
121-32-4	3-Ethoxy-4-hydroxybenzaldehyde	1.55	87.6	0.40
121-33-5	Vanillin	1.05	83.8	0.78
121-69-7	N,N-Dimethylaniline	2.17	64.1	-0.09
121-73-3	1-Chloro-3-nitrobenzene	2.46	18.7	0.33
121-75-5	Malathion	2.29	14.1	0.91
121-87-9	2-Chloro-4-nitroaniline	2.12	20	0.61
122-03-2	p-Isopropyl benzaldehyde	3.17	6.62	0.20
122-39-4	Diphenylamine	3.29	3.79	0.40
122-99-6	2-Phenoxyethanol	1.10	344	0.08
123-07-9	4-Ethylphenol	2.55	10.4	0.41
123-15-9	2-Methylvaleraldehyde	1.73	18.8	0.71
123-54-6	2,4-Pentanedione	0.05	135	1.18
123-66-0	Ethyl hexanoate	2.83	8.9	0.32
123-72-8	Butanal	0.82	14.7	1.39
123-86-4	Butyl acetate	1.85	18	0.70

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
123-91-1	1,4-Dioxane	-0.32	10300	-0.47
124-22-1	Dodecylamine	4.76	0.103	0.84
126-73-8	Tributyl phosphate	3.82	9.48	-0.22
126-81-8	5,5-Dimethyl-1,3-cyclohexanedione	1.30	11500	-1.59
127-00-4	1-Chloro-2-propanol	0.53	245	0.52
127-18-4	Tetrachloroethylene	2.97	16.5	0.01
127-66-2	2-Phenyl-3-butyn-2-ol	1.67	113	0.14
128-37-0	2,6-Di-tert-butyl-4-methylphenol	5.03	0.364	0.16
13071-79-9	Terbufos (counter)	4.49	0.0133	2.14
13209-15-9	alpha,alpha,alpha',alpha'-Tetrabromo-o-xylene	4.31	0.439	0.93
132-64-9	Dibenzofuran	4.05	1.5	0.20
133-11-9	Phenyl 4-aminosalicylate	2.95	4.77	0.70
134-62-3	N,N-Diethyl-m-toluamide	2.26	110	-0.20
13608-87-2	2',3',4'-Trichloroacetophenone	3.61	2	0.55
13909-73-4	2',3',4'-Trimethoxyacetophenone	1.18	199	0.44
13952-84-6	(+-)-sec-Butylamine	0.76	275	0.17
140-31-8	1-(2-Aminoethyl)piperazine	-1.57	2190	1.36
14064-10-9	Diethyl chloromalonate	1.08	0.95	2.81
141-03-7	Dibutyl succinate	3.35	4.47	0.42
141-28-6	Diethyl adipate	2.37	18.2	0.52
141-43-5	2-Aminoethanol	-1.61	2070	1.09
141-78-6	Ethyl acetate	0.86	230	0.25
141-91-3	2,6-Dimethyl morpholine	0.28	387	0.60
141-93-5	m-Diethylbenzene	4.07	4.15	-0.36
142-28-9	1,3-Dichloropropane	2.32	111	-0.47
142-62-1	Hexanoic acid	2.05	320	-0.71
142-92-7	Hexyl acetate	2.83	4.4	0.63
142-96-1	Butyl ether	3.01	32.3	-0.42
143-08-8	1-Nonanol	3.30	5.7	0.15
143-16-8	Di-n-hexylamine	4.74	0.78	-0.02
14321-27-8	N-Ethylbenzylamine	2.03	57.1	0.12
14548-45-9	4-Bromophenyl 3-pyridyl ketone	2.85	20.4	0.21
14548-46-0	4-Benzoylpyridine	1.96	103	0.05
1482-15-1	3,4-Dimethyl-1-pentyn-3-ol	1.36	205	0.01
1484-13-5	N-Vinylcarbazole	4.19	0.00321	2.82
1484-26-0	3-Benzyloxyaniline	2.86	9.15	0.43
148-53-8	o-Vanillin	1.83	2.4	1.71
150-19-6	3-Methoxyphenol	1.59	74	0.32
15045-43-9	2,2,5,5-Tetramethyltetrahydrofuran	2.68	168	-0.88
150-76-5	4-Methoxyphenol	1.59	110	0.15
150-78-7	p-Dimethoxybenzene	2.15	117	-0.28
15128-82-2	3-Hydroxy-2-nitropyridine	0.72	167	0.70
1563-66-2	Carbofuran	2.30	0.843	1.95
15972-60-8	Alachlor	3.37	4.99	0.42
16245-79-7	4-Octylaniline	5.06	0.12	0.59
1634-04-4	tert-Butyl methyl ether	1.43	672	-0.66
1647-16-1	1,9-Decadiene	4.98	0.29	0.09
16752-77-5	Methomyl	0.61	2.11	2.75
16879-02-0	6-Chloro-2-pyridinol	1.72	214	-0.23
1689-82-3	p-Phenylazophenol	3.63	1.19	0.70
1689-83-4	3,5-Diiodo-4-hydroxybenzonitrile	3.94	6.79	-0.03
1689-84-5	3,5-Dibromo-4-hydroxybenzonitrile	3.39	12.6	0.01
1740-19-8	Dehydroabietic acid	6.52	2.1	-1.65
1745-81-9	2-Allylphenol	2.91	15	0.00
1746-23-2	t-Butylstyrene	4.80	0.49	0.07
17584-12-2	3-Amino-5,6-dimethyl-1,2,4-triazine	-0.05	952	0.50
1761-61-1	5-Bromosalicylaldehyde	2.90	1.3	1.25
17754-90-4	4-(Diethylamino)salicylaldehyde	2.82	5.35	0.68
18368-63-3	6-Chloro-2-picoline	2.00	232	-0.49
1871-57-4	3-Chloro-2-chloromethyl-1-propene	2.73	0.19	2.01
1891-95-8	3,5-Dichloro-4-hydroxybenzonitrile	2.90	24.3	-0.05
19549-98-5	3,6-Dimethyl-1-heptyn-3-ol	2.34	48.9	-0.04
1962-75-0	Di-n-butylterephthalate	4.61	0.59	0.38

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
1965-09-9	4,4'-Dihydroxydiphenyl ether	3.09	5.78	0.45
2008-58-4	2,6-Dichlorobenzamide	0.90	469	0.25
2016-57-1	n-Decylamine	3.78	1.03	0.55
2032-59-9	Aminocarb	1.90	1.95	1.88
2034-22-2	2,4,5-Tribromoimidazole	2.73	6.13	0.89
20662-84-4	2,4,5-Trimethyloxazole	1.86	449	-0.73
2104-64-5	O-Ethyl O-(p-nitrophenyl phenyl)phosphonothioate	4.47	0.0786	1.43
2117-11-5	(+-)-4-Pentyn-2-ol	0.49	35.1	1.34
2138-22-9	4-Chlorocatechol	1.68	1.58	1.99
2150-47-2	Methyl 2,4-dihydroxybenzoate	2.12	45.7	0.24
2176-62-7	Pentachloropyridine	4.03	0.47	0.89
22037-97-4	4,7-Dithiadecane	3.46	7.53	-0.01
22104-62-7	4-Dimethylamino-3-methyl-2-butanone	-0.12	8.5	2.63
2216-51-5	(1R,2S,5R)-(-)-menthol	3.38	18.9	-0.40
2232-08-8	1-(p-Toluenesulfonyl)imidazole	1.92	41.8	0.56
2234-16-4	2',4'-Dichloroacetophenone	2.96	13	0.17
2243-27-8	n-Octyl cyanide	3.29	5.25	0.17
22726-00-7	m-Bromobenzamide	1.63	92.6	0.40
23135-22-0	Oxamyl	-1.20	6.78	3.81
2357-47-3	alpha,alpha,alpha-4-Tetrafluoro-m-toluidine	2.24	30.1	0.36
2362-61-0	trans-2-Phenyl-1-cyclohexanol	3.27	44.4	-0.63
2370-63-0	2-Ethoxyethyl methacrylate	1.49	27.7	0.93
2416-94-6	2,3,6-Trimethylphenol	3.15	8.2	0.08
2437-25-4	n-Undecyl cyanide	4.77	0.43	0.21
2439-77-2	o-Methoxybenzamide	0.28	120	1.23
2447-79-2	2,4-Dichlorobenzamide	1.29	95.6	0.63
24544-04-5	2,6-Diisopropylaniline	3.99	15.3	-0.74
2455-24-5	Tetrahydrofurfuryl methacrylate	1.80	34.7	0.62
2460-49-3	4,5-Dichloroguaiacol	2.63	4.48	0.91
2495-37-6	Benzyl methacrylate	2.98	4.67	0.57
2499-95-8	hexyl acrylate	3.18	1.11	0.99
25154-52-3	Nonylphenol (mixed)	5.99	0.14	-0.18
2626-83-7	p-(tert-butyl)-Phenyl-N-methylcarbamate	3.08	9.99	0.23
271-89-6	2,3-Benzofuran	2.54	14.1	0.27
2759-28-6	1-Benzylpiperazine	1.12	47.4	1.04
280-57-9	1,4-Diazabicyclo[2.2.2]octane	-0.49	1730	0.55
281-23-2	Adamantane	3.94	0.281	0.92
2859-67-8	3-(3-Pyridyl)-1-propanol	0.87	150	0.62
2869-34-3	Tridecylamine	5.25	0.0654	0.69
2894-51-1	2-Amino-4'-chlorobenzophenone	3.69	2.12	0.47
2905-69-3	Methyl 2,5-dichlorobenzoate	3.12	14	0.05
2921-88-2	Chlorpyrifos (Dursban)	5.11	0.318	0.36
29553-26-2	2-Methyl-3,3,4,4-tetrafluoro-2-butanol	1.50	582	-0.40
2973-76-4	5-Bromovanillin	1.94	59.6	0.41
298-04-4	Disulfoton	4.07	2.73	0.14
30030-25-2	Chloromethyl styrene	3.70	0.31	1.12
3066-71-5	Cyclohexyl acrylate	3.00	1.48	1.00
3126-90-7	Di-n-butylisophthlate	4.61	0.899	0.20
314-40-9	Bromacil	1.68	186	0.17
31502-57-5	2-chloroethyl-N-cyclohexyl carbamate	2.97	35	-0.23
3206-31-3	Triethyl nitrilotricarboxylate	2.49	13.3	0.63
329-71-5	2,5-Dinitrophenol	1.73	3.35	1.72
330-54-1	Diuron	2.67	14.2	0.46
330-93-8	p-Fluorophenyl ether	4.45	1.13	0.10
333-41-5	Diazinon	3.86	9.34	-0.19
34274-04-9	N-(3-Methoxypropyl)-3,4,5-trimethoxybenzylamine	1.26	136	0.65
3428-24-8	4,5-Dichlorocatechol	2.32	0.89	1.82
34723-82-5	2-(Bromomethyl)tetrahydro-2H-pyran	2.19	205	-0.44
3481-20-7	2,3,5,6-Tetrachloroaniline	3.65	0.27	1.40
350-46-9	1-Fluoro-4-nitrobenzene	2.01	28.4	0.46
3558-69-8	2,6-Diphenylpyridine	4.33	0.21	0.97
368-77-4	alpha,alpha,alpha-Trifluoro-m-tolunitrile	2.50	47.7	-0.07
3698-83-7	1,3-Dichloro-4,6-dinitrobenzene	2.92	0.0455	2.76

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
371-40-4	4-Fluoroaniline	1.28	16.9	1.16
37529-30-9	4-Decylaniline	6.04	0.0621	0.15
387-45-1	2-Chloro-6-fluorobenzaldehyde	2.56	9.4	0.55
39145-47-6	p-Chlorophenyl-o-nitrophenyl ether	3.67	1.92	0.56
3923-52-2	1,1-Diphenyl-2-propyn-1-ol	2.88	11.1	0.35
393-39-5	alpha,alpha,alpha-4-Tetrafluoro-o-toluidine	2.24	29.6	0.36
3944-76-1	2,3-Dimethylvaleraldehyde	2.14	16	0.51
39905-57-2	4-Hexyloxyaniline	3.61	3.02	0.30
4117-14-0	2-Decyn-1-ol	3.07	1.07	1.08
42087-80-9	Methyl 4-chloro-2-nitrobenzoate	2.29	27.6	0.43
4214-79-3	5-Chloro-2-pyridinol	1.72	1140	-0.95
42454-06-8	5-Hydroxy-2-nitrobenzaldehyde	1.63	41.9	0.66
4253-89-8	Isopropyl disulfide	3.69	8.31	-0.31
4460-86-0	2,4,5-Trimethoxybenzaldehyde	1.44	49.4	0.81
446-52-6	2-Fluorobenzaldehyde	1.91	1.35	1.80
447-60-9	alpha,alpha,alpha-Trifluoro-o-tolunitrile	2.50	42.3	-0.02
454-89-7	alpha,alpha,alpha-Trifluoro-m-tolualdehyde	2.67	0.925	1.52
459-59-6	4-Fluoro-N-methylaniline	1.82	38.4	0.43
464-45-9	[(1S)-endo]-(-)-Borneol	2.85	63.2	-0.51
464-48-2	(1S)-(-)-Camphor	3.04	17.1	-0.10
4655-34-9	Isopropyl methacrylate	2.18	37.9	0.16
470-82-6	Cineole	3.13	102	-0.94
471-77-2	Neoabietic acid	6.59	1.49	-1.55
4798-44-1	1-Hexen-3-ol	1.61	30.4	0.60
4901-51-3	2,3,4,5-Tetrachlorophenol	4.09	0.41	0.87
4916-57-8	1,2-bis(4-Pyridyl)ethane	2.36	151	-0.43
496-16-2	2,3-Dihydrobenzofuran	2.51	81.7	-0.47
497-37-0	exo-Norborneol	1.53	228	-0.17
498-66-8	Norbornylene	2.85	9.98	0.07
499-83-2	2,6-Pyridinedicarboxylic acid	0.57	322	0.61
500-22-1	3-Pyridinecarboxaldehyde	0.52	16.4	1.75
50-06-6	Phenobarbital	1.33	483	-0.02
502-56-7	5-Nonanone	2.71	31	-0.13
51-28-5	2,4-Dinitrophenol	1.73	10.9	1.21
513-81-5	2,3-Dimethyl-1,3-butadiene	3.13	6.91	-0.05
514-10-3	Abietic acid	6.46	2.38	-1.65
51630-58-1	Fenvalerate	6.76	0.00508	0.93
51-79-6	Urethane	-0.02	5240	-0.40
5217-47-0	1,3-Diethyl-2-thiobarbituric acid	1.03	4510	-0.82
525-82-6	Flavone	3.51	3.49	0.38
52645-53-1	Permethrin	7.43	0.016	-0.13
527-60-6	2,4,6-Trimethylphenol	3.15	13	-0.12
529-19-1	o-Tolunitrile	2.09	44.8	0.12
529-20-4	o-Tolualdehyde	2.26	52.9	-0.08
5292-45-5	Dimethyl nitroterephthalate	1.48	6.53	1.74
5331-91-9	5-Chloro-2-mercaptobenzothiazole	3.51	3.21	0.38
534-52-1	4,6-Dinitro-o-cresol	2.27	1.73	1.62
5372-81-6	Dimethyl aminoterephthalate	2.10	8.93	1.06
538-68-1	Amylbenzene	4.50	1.7	-0.27
5395-75-5	3,6-Dithiaoctane	2.48	60.3	-0.21
540-88-5	tert-Butyl acetate	1.74	327	-0.47
541-73-1	1,3-Dichlorobenzene	3.28	8.03	0.02
542-75-6	1,3-Dichloropropene	2.29	0.239	2.21
544-40-1	n-Butyl sulfide	3.87	3.58	-0.10
54576-32-8	3,8-Dithiadecane	3.46	6.06	0.09
5465-65-6	4'-Chloro-3'-nitroacetophenone	2.14	5.51	1.22
55-21-0	Benzamide	0.74	661	0.03
552-41-0	2'-Hydroxy-4'-methoxyacetophenone	2.05	69.5	0.11
552-89-6	o-Nitrobenzaldehyde	1.53	14.4	1.16
555-16-8	4-Nitrobenzaldehyde	1.53	10.1	1.32
55792-61-5	2'-(Octyloxy)-acetanilide	4.05	0.45	0.92
5600-21-5	2-Amino-4-chloro-6-methylpyrimidine	1.07	141	0.51
56108-12-4	p-(tert-Butyl)benzamide	2.65	31.9	0.00

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
56348-39-1	4,9-Dithiadodecane	4.44	2.99	-0.32
56348-40-4	2,9-Dithiadecane	3.46	10.1	-0.14
563-80-4	3-Methyl-2-butanone	0.67	864	-0.18
5673-07-4	2,6-Dimethoxytoluene	2.70	20.2	0.09
5683-33-0	2-Dimethylaminopyridine	1.62	127	0.05
57-14-7	1,1-Dimethyl hydrazine	-1.19	7.87	3.17
573-56-8	2,6-Dinitrophenol	1.73	39.8	0.65
57-43-2	Amobarbital	2.00	85.3	0.19
58-08-2	Caffeine	0.16	151	1.33
5813-64-9	2,2-Dimethyl-1-propylamine	1.21	475	-0.34
58-27-5	2-Methyl-1,4-naphthoquinone	2.21	0.11	2.80
5835-26-7	Isopimaric acid	6.45	0.871	-1.20
583-53-9	1,2-Dibromobenzene	3.77	4.06	0.14
58-90-2	2,3,4,6-Tetrachlorophenol	4.09	1.03	0.47
589-09-3	N-Allylaniline	2.47	36	-0.03
589-16-2	4-Ethylaniline	2.11	73	-0.10
590-86-3	Isovaleraldehyde	1.23	3.25	1.80
591-78-6	2-Hexanone	1.24	428	-0.26
5922-60-1	2-Amino-5-chlorobenzonitrile	1.82	28.5	0.64
592-46-1	2,4-Hexadiene	2.86	20	-0.30
593-08-8	2-Tridecanone	4.68	0.359	0.40
59-50-7	4-Chloro-3-methyl phenol	2.70	5.48	0.63
596-85-0	Manool	7.09	0.12	-0.87
598-74-3	1,2-Dimethylpropylamine	1.18	284	-0.10
600-36-2	2,4-Dimethyl-3-pentanol	2.09	163	-0.45
60-29-7	Diethyl ether	1.05	2560	-1.02
607-00-1	N,N-Diphenylformamide	1.91	30.4	0.65
607-81-8	Diethyl benzylmalonate	3.02	5.43	0.63
608-71-9	Pentabromophenol	5.96	0.0928	0.36
609-23-4	2,4,6-Triiodophenol	5.01	1.21	-0.02
61096-84-2	4-(Hexyloxy)-m-anisaldehyde	3.81	2.67	0.29
613-45-6	2,4-Dimethoxybenzaldehyde	1.87	20.1	0.79
614-80-2	2-Acetamidophenol	0.62	27.1	1.61
615-65-6	2-Chloro-4-methylaniline	2.27	36	0.15
616-86-4	4-Ethoxy-2-nitroaniline	2.59	26.1	0.15
6175-49-1	2-Dodecanone	4.18	1.18	0.24
619-50-1	Methyl p-nitrobenzoate	1.65	23.7	0.93
619-80-7	4-Nitrobenzamide	0.56	133	1.00
6203-18-5	4-Dimethylaminocinnamaldehyde	2.00	6.43	1.21
620-88-2	4-Nitrophenyl phenyl ether	3.87	2.65	0.20
621-08-9	Benzyl sulfoxide	2.19	80.2	0.08
621-42-1	3-Acetamidophenol	0.27	1130	0.26
622-40-2	4-(2-Hydroxyethyl)morpholine	-1.32	2710	1.08
623-25-6	alpha,alpha'-Dichloro-p-xylene	3.60	0.039	2.16
62-53-3	Aniline	1.08	105	0.44
625-86-5	2,5-Dimethylfuran	2.46	71.1	-0.46
6284-83-9	1,3,5-Trichloro-2,4-dinitrobenzene	3.56	0.222	1.62
628-76-2	1,5-Dichloropentane	3.30	25.2	-0.51
629-04-9	1-Bromoheptane	4.12	1.47	0.18
629-19-6	Propyl disulfide	3.84	2.56	0.09
629-40-3	1,6-Dicyanohexane	1.33	528	-0.29
63-25-2	Carbaryl (sevin)	2.35	8.75	0.86
634-67-3	2,3,4-Trichloroaniline	3.01	3.63	0.70
635-93-8	5-Chlorosalicylaldehyde	2.65	0.77	1.56
6361-21-3	2-Chloro-5-nitrobenzaldehyde	2.17	3.88	1.32
64-17-5	Ethanol	-0.14	14700	-1.04
645-56-7	4-Propylphenol	3.04	11	0.04
65337-13-5	dl-3-Butyn-2-ol	0.00	11.7	2.13
653-37-2	Pentafluorobenzaldehyde	2.71	1.1	1.46
65-45-2	2-Hydroxybenzamide	1.03	101	0.67
6575-09-3	2-Chloro-6-methylbenzonitrile	2.73	15.1	0.20
6602-32-0	2-Bromo-3-pyridinol	1.21	469	-0.04
66-25-1	Hexanal	1.80	17.5	0.68

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
6636-78-8	2-Chloro-3-pyridinol	0.97	622	-0.10
66-76-2	Dicumarol	1.92	5.11	1.65
67-36-7	p-Phenoxybenzaldehyde	3.77	4.6	0.01
67-56-1	Methanol	-0.63	29400	-1.11
67-63-0	2-Propanol	0.28	8650	-1.03
67-64-1	Acetone	-0.24	7140	-0.55
67-66-3	Chloroform	1.52	70.7	0.38
67-68-5	Methyl sulfoxide	-1.22	34000	-0.32
67-72-1	Hexachloroethane	4.03	1.42	0.39
683-72-7	2,2-Dichloroacetamide	-0.09	241	1.15
6921-29-5	Tripropargylamine	0.67	296	0.47
693-16-3	1-Methyl heptylamine	2.73	5.2	0.59
693-54-9	2-Decanone	3.20	4.83	0.33
693-65-2	Pentyl ether	4.00	3.13	-0.11
693-93-6	4-Methyloxazole	0.76	1390	-0.47
693-98-1	2-Methylimidazole	0.61	286	0.33
6948-86-3	N,N-bis(2,2-Diethoxyethyl)methylamine	0.78	635	0.35
69723-94-0	1-Benzylpyridinium 3-sulfonate	-2.62	2410	2.43
69770-23-6	3-(4-tert-Butylphenoxy)benzaldehyde	5.68	0.369	-0.30
700-58-3	2-Adamantanone	2.59	60.8	-0.30
70124-77-5	Flucythrinate	6.56	0.00019	2.54
70-30-4	2,2'-Methylene bis(3,4,6-trichlorophenol)	6.92	0.021	0.17
706-14-9	gamma-Decanolactone	2.57	18	0.29
70-69-9	4'-Aminopropiophenone	1.25	146	0.37
708-76-9	4,6-Dimethoxy-2-hydroxybenzaldehyde	2.17	2.68	1.47
709-98-8	Propanil	2.88	8.59	0.48
71-23-8	1-Propanol	0.35	4550	-0.81
71-36-3	n-Butanol	0.84	1730	-0.68
71-41-0	1-Pentanol	1.33	472	-0.43
71-43-2	Benzene	1.99	17.6	0.43
71-55-6	1,1,1-Trichloroethane	2.68	47.4	-0.32
71862-02-7	3'-Chloro-o-formotoluidide	2.32	46.6	0.08
7209-38-3	1,4-bis(3-Aminopropyl)piperazine	-1.35	3100	1.23
7212-44-4	3-Hydroxy-3,7,11-trimethyl-1,6,10-dodecatriene	5.68	1.43	-0.95
7307-55-3	n-Undecylamine	4.27	0.211	0.89
732-26-3	2,4,6-Tri-tert-butylphenol	6.39	0.0609	-0.06
7383-19-9	1-Heptyn-3-ol	1.47	1.76	1.99
75-05-8	Acetonitrile	-0.15	1640	-0.13
75-07-0	Ethanal	-0.17	33.8	1.60
75-09-2	Dichloromethane	1.34	330	-0.30
75-47-8	Iodoform	3.03	2.92	1.09
75-65-0	2-Methyl-2-propanol	0.73	6410	-1.16
75-89-8	2,2,2-Trifluoroethanol	0.27	119	1.06
75-97-8	3,3-Dimethyl-2-butanone	1.13	87	0.52
76-01-7	Pentachloroethane	3.11	7.53	0.32
760-23-6	3,4-Dichloro-1-butene	2.60	8.17	0.48
761-65-9	N,N-Dibutylformamide	2.01	89.3	0.01
764-01-2	2-Butyn-1-ol	0.13	10.1	2.09
764-13-6	2,5-Dimethyl-2,4-hexadiene	3.95	3.78	-0.31
768-94-5	1-Adamantanamine	2.43	25	0.21
769-28-8	3-Cyano-4,6-dimethyl-2-hydroxypyridine	2.27	157	-0.47
771-60-8	2,3,4,5,6-Pentafluoroaniline	2.08	37.2	0.40
77-71-4	5,5-Dimethylhydantoin	-0.27	16500	-0.55
77-74-7	3-Methyl-3-pentanol	1.71	672	-0.82
77-75-8	3-Methyl-1-pentyn-3-ol	0.94	1220	-0.49
78-27-3	1-Ethynyl-cyclohexanol	1.81	256	-0.39
78-51-3	Tris(2-butoxyethyl) phosphate	3.00	11.2	0.53
786-19-6	Carbophenothion	5.44	0.24	0.21
78-83-1	2-Methyl-1-propanol	0.77	1430	-0.54
78-87-5	1,2-Dichloropropane	2.25	127	-0.48
78-90-0	1,2-Diaminopropane	-1.20	1010	1.16
78-92-2	2-Butanol	0.77	3670	-0.95
78-93-3	2-Butanone	0.26	3220	-0.51

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
78-96-6	1-Amino-2-propanol	-1.19	2520	0.76
79-00-5	1,1,2-Trichloroethane	2.01	81.6	-0.02
79-01-6	Trichloroethylene	2.47	44.1	-0.13
79124-76-8	3-(3,4-Dichlorophenoxy)benzaldehyde	5.06	0.299	0.30
791-28-6	Triphenylphosphine oxide	2.87	53.7	-0.20
79-20-9	Methyl acetate	0.37	357	0.37
79-34-5	1,1,2,2-Tetrachloroethane	2.19	20.3	0.54
79-77-6	beta-Ionone	4.42	5.1	-0.57
79-95-8	4,4'-Isopropylidenebis(2,6-dichlorophenol)	6.22	1.33	-1.12
80-46-6	p-tert-Pentylphenol	3.91	2.6	0.06
80-52-4	1,8-Diamino-p-menthane	1.90	65.2	0.27
8065-48-3	Demeton O,S	1.99	16	0.99
81-19-6	alpha,alpha-2,6-Tetrachlorotoluene	4.26	0.97	0.36
818-61-1	2-Hydroxyethyl acrylate	-0.25	4.81	2.93
818-72-4	1-Octyn-3-ol	1.96	0.413	2.29
821-55-6	2-Nonanone	2.71	15.2	0.18
822-86-6	trans-1,2-Dichlorocyclohexane	3.54	18.4	-0.53
831-82-3	p-Phenoxyphenol	3.57	4.95	0.10
83-32-9	Acenaphthene	4.15	1.73	0.02
83-34-1	3-Methylindole	2.60	8.84	0.47
83-79-4	Rotenone	4.31	0.00521	2.82
84-62-8	Diphenyl phthalate	4.10	0.0799	1.71
84-66-2	Diethyl phthalate	2.65	31.8	0.10
84-74-2	Di-n-butylorthophthalate	4.61	0.999	0.15
86-50-0	Azinphos-methyl	2.53	0.0641	3.05
868-77-9	2-Hydroxyethyl methacrylate	0.30	227	0.87
87-17-2	Salicylanilide	3.30	3.94	0.48
872-31-1	3-Bromothiophene	2.70	6.2	0.64
874-42-0	2,4-Dichlorobenzaldehyde	3.00	1.8	0.97
87-68-3	Hexachloro-1,3-butadiene	4.72	0.09	1.08
87-86-5	Pentachlorophenol	4.74	0.243	0.65
88-06-2	2,4,6-Trichlorophenol	3.45	4.9	0.23
882-33-7	Phenyl disulfide	4.31	0.11	1.24
88-30-2	3-Trifluoromethyl-4-nitrophenol	2.87	9.13	0.44
88-68-6	Anthranilamide	0.44	395	0.54
88-75-5	2-Nitrophenol	1.91	160	-0.22
88-85-7	2-sec-Butyl-4,6-dinitrophenol (dinoseb)	3.67	0.536	1.10
90-02-8	Salicylaldehyde	2.01	2.3	1.49
90-15-3	1-Naphthol	2.69	4.63	0.72
90-43-7	2-Phenylphenol	3.28	6.14	0.20
90-59-5	3,5-Dibromosalicylaldehyde	3.79	0.851	0.87
91-20-3	Naphthalene	3.17	6.14	0.17
91-22-5	Quinoline	2.14	77.8	-0.12
91-65-6	N,N-Diethylcyclohexylamine	3.29	21.4	-0.39
91-66-7	N,N-Diethylaniline	3.15	16.4	-0.18
91-88-3	2-(N-Ethyl-m-toluidino)ethanol	2.24	52.9	0.11
920-66-1	1,1,1,3,3,3-Hexafluoro-2-propanol	1.11	244	0.31
924-41-4	1,5-Hexadien-3-ol	1.48	38.1	0.59
927-74-2	3-Butyn-1-ol	0.07	36.1	1.58
928-96-1	cis-3-Hexen-1-ol	1.61	381	-0.50
928-97-2	trans-3-Hexen-1-ol	1.61	271	-0.35
932-16-1	2-Acetyl-1-methylpyrrole	1.11	157	0.37
93-91-4	1-Benzoylacetone	0.61	1.1	3.04
939-23-1	4-Phenylpyridine	2.57	16.1	0.30
94-09-7	Ethyl p-aminobenzoate	1.80	35.7	0.59
945-51-7	Phenyl sulfoxide	2.07	87.4	0.08
94-62-2	Piperine (aliphatic)	3.69	7.85	0.00
95-01-2	2,4-Dihydroxybenzaldehyde	1.53	13.1	1.16
95-47-6	o-Xylene	3.09	16.3	-0.28
95-48-7	o-Cresol	2.06	13.9	0.61
95-50-1	1,2-Dichlorobenzene	3.28	9.41	-0.05
95-51-2	2-Chloroaniline	1.72	5.74	1.34
95-52-3	2-Fluorotoluene	2.74	19.4	-0.06

CAS	Compound	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)
95-57-8	2-Chlorophenol	2.16	11.4	0.70
95-63-6	1,2,4-Trimethylbenzene	3.63	7.72	-0.33
95-75-0	3,4-Dichlorotoluene	3.83	2.91	0.07
95-76-1	3,4-Dichloroaniline	2.37	7.57	0.81
96-05-9	Allyl methacrylate	2.12	0.99	1.78
96-13-9	2,3-Dibromopropanol	0.96	71	1.08
96-17-3	2-Methylbutyraldehyde	1.23	9.99	1.31
96-18-4	1,2,3-Trichloropropane	2.50	57.6	-0.22
96-22-0	3-Pentanone	0.75	1540	-0.49
96-29-7	2-Butanone oxime	1.69	843	-0.97
96-80-0	2-(Diisopropylamino)ethanol	0.88	201	0.51
97-02-9	2,4-Dinitroaniline	1.84	14.8	0.99
97-23-4	2,2'-Methylenebis(4-chlorophenol)	4.34	0.309	0.86
98434-34-5	5-Bromo-2-nitrovanillin	2.34	73.4	0.08
98-54-4	p-tert-Butylphenol	3.42	5.15	0.11
98-82-8	Isopropylbenzene	3.45	6.32	-0.10
98-86-2	Acetophenone	1.67	162	-0.10
98-95-3	Nitrobenzene	1.81	119	-0.07
99-03-6	m-Aminoacetophenone	0.76	382	0.30
99-08-1	m-Nitrotoluene	2.36	25.6	0.21
999-61-1	2-Hydroxypropyl acrylate	0.17	3.38	2.80
99-97-8	N,N-Dimethyl-p-toluidine	2.72	48.9	-0.36

S2. Additional information on the test set

Fish acute toxicity data for diverse fish species were collected from the Hommel compendium of hazardous substances.[7] The Hommel dataset contains supplier information, mainly from material safety data sheets and registration dossiers published by the European Chemicals Agency (ECHA). The quality of the data is variable due to diverse fish species and test conditions.[8] The external test set was limited to the 96 h LC_{50} data [mmol/L] (n = 378: 258 baseline, 120 excess) that were available for 316 discrete organic compounds with a range in molecular weight from 30.0 to 406.9 g/mol and log K_{ow} from -4.15 to 7.95. The log K_{ow} values were calculated.[2] If additional measured log K_{ow} data were available the mean value was used. 96 h LC_{50} data from the EPAFHM[1] in the Hommel dataset were excluded from the test set. If multiple 96 h LC_{50} data were available for the same compound, all of them remained in the external test set as to be able to see if all or only some of these real-life data are covered by the classification scheme (Table S2).

Chemicals were grouped as either baseline or excess toxicants based on their experimental fish acute toxicity data relative to a log K_{ow}-dependent baseline QSAR[3] for acute fish toxicities [96-h LC_{50} (*Pimephales promelas*): log $1/LC_{50}$ [mmol/L] = 0.79 log K_{ow} - 1.35, where n = 147, r = 0.92, s = 0.40; n is the number of observations, r is the correlation coefficient and s is the standard deviation of the residuals]. The toxicity estimates were compared to the available experimental fish acute toxicity data. If calculated and experimental toxicity data agreed within a factor of 10, i.e. residuals (log $1/LC_{50\ exp}$ - log $1/LC_{50\ calc}$) <1 log unit, chemicals were considered baseline toxicants. Excess toxicity as introduced by Lipnick[4, 5] refers to enhanced effects of compounds relative to their baseline toxicity. Excess toxicity significantly, at least 10-times, exceeds the calculated baseline toxicity. Deviations larger than a factor of 10, i.e. residuals (log $1/LC_{50\ exp}$ - log $1/LC_{50\ calc}$) >1 log unit, prompted assignment of excess toxicity. Note that excess toxicities are based on a formal comparison of the experimental and calculated numeric values and may be due to diverse MOA related to the chemical reactivities of the toxicants with biological targets.[6]

Table S2: Test set of fish acute toxicity data.

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
50-00-0	Formaldehyde	excess	0.56	41	0.77	*Danio rerio*
51-28-5	2,4-Dinitrophenol	excess	1.73	8.6	1.31	--
55-38-9	Fenthion	excess	4.09	1.52	0.39	--
56-18-8	N-(3-Aminopropyl)-1,3-propanediamine	excess	-1.20	230	2.05	*Leuciscus idus*
56-81-5	1,2,3-Propanetriol	not classified	-1.71	54000	-0.07	*Oncorhynchus mykiss*
57-24-9	Strychnine	not classified	1.89	0.91	2.42	--
57-55-6	1,2-Propanediol	baseline	-0.85	46500	-0.76	*Pimephales promelas*
				54900	-0.84	*Pimephales promelas*
				51600	-0.81	*Oncorhynchus mykiss*
58-08-2	Caffeine	not classified	0.03	87	1.67	*Leuciscus idus*
59-50-7	4-Chloro-3-methylphenol	baseline	2.86	0.917	1.28	*Oncorhynchus mykiss*
60-00-4	EDTA	not classified	-3.86	135	4.73	*Lepomis macrochirus*
60-12-8	Phenylethanol	baseline	1.47	340	-0.25	*Leuciscus idus*
60-24-2	2-Mercaptoethanol	excess	-0.13	37	1.78	*Leuciscus idus*
60-51-5	Dimethoate	excess	0.71	30.2	1.67	*Oncorhynchus mykiss*
62-53-3	Benzenamine	not classified	1.08	10.6	1.44	*Oncorhynchus mykiss*
62-56-6	Thiourea	excess	-1.12	10000	0.11	*Danio rerio*
64-17-5	Ethanol	baseline	-0.23	13000	-0.92	*Oncorhynchus mykiss*
65-85-0	Benzoic acid	baseline	1.87	44.6	0.31	*Lepomis macrochirus*
				47.3	0.28	*Oncorhynchus mykiss*
67-63-0	2-Propanol	baseline	0.17	9640	-0.99	*Pimephales promelas*
67-64-1	2-Propanone	baseline	-0.24	6070	-0.48	*Salvelinus fontinalis*

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
68-12-2	N,N-Dimethylformamide	excess	-0.93	9800	-0.04	*Oncorhynchus mykiss*
				7100	0.10	*Lepomis macrochirus*
				78.2	2.06	*Pimephales promelas*
69-72-7	Salicylic acid	baseline	2.27	1380	-1.44	*Pimephales promelas*
70-30-4	Hexachlorophene	not classified	7.23	0.021	-0.07	--
71-23-8	n-Propanol	baseline	0.28	4630	-0.75	*Pimephales promelas*
71-36-3	n-Butanol	baseline	0.84	1380	-0.58	*Pimephales promelas*
71-43-2	Benzene	baseline	2.06	5.3	0.89	*Oncorhynchus mykiss*
74-87-3	Chloromethane	baseline	1.09	730	-0.67	*Lepomis macrochirus*
75-01-4	Chloroethene	baseline	1.62	210	-0.46	*Danio rerio*
75-08-1	Ethanethiol	excess	1.27	2.4	1.76	*Oncorhynchus mykiss*
75-09-2	Dichloromethane	baseline	1.34	193	-0.07	*Pimephales promelas*
75-12-7	Formamide	not classified	-1.22	6570	0.15	*Leuciscus idus*
75-21-8	Oxirane	excess	-0.05	84	1.11	*Pimephales promelas*
75-31-0	2-Propanamine	not classified	-0.12	40	1.61	*Oncorhynchus mykiss*
75-50-3	Trimethylamine	baseline	0.04	25	1.69	*Leuciscus idus*
75-56-9	Propylenoxid	excess	0.37	89	0.87	*Mugil cephalus*
				52	1.11	*Oncorhynchus mykiss*
75-64-9	tert-Butylamine	not classified	0.56	270	0.34	*Oncorhynchus mykiss*
				28	1.32	*Oncorhynchus mykiss*
76-22-2	Camphor	baseline	3.04	17	-0.10	*Pimephales promelas*
				110	-0.91	*Pimephales promelas*
78-70-6	Linalool	not classified	3.04	31	-0.35	*Leuciscus idus*
78-84-2	2-Methylpropanal	excess	0.74	23	1.26	*Pimephales promelas*
78-96-6	1-Amino-2-propanol	not classified	-1.06	340	1.53	*Leuciscus idus*
				210	1.74	*Carassius auratus*
78-98-8	Pyruvic aldehyde	excess	-1.28	1000	1.22	*Leuciscus idus*
79-00-5	1,1,2-Trichloroethane	baseline	2.01	41	0.27	--
				81.6	-0.02	--
79-01-6	Trichloroethene	baseline	2.47	41	-0.10	*Pimephales promelas*
79-06-1	Acrylamide	excess	-1.04	66	2.21	*Poecilia reticulata*
				200	1.72	*Lepomis macrochirus*
				220	1.68	*Oncorhynchus mykiss*
				240	1.65	*Pimephales promelas*
79-10-7	2-Propenoic acid	excess	0.44	27	1.43	*Oncorhynchus mykiss*
79-11-8	Chloroacetic acid	excess	0.34	370	0.49	*Danio rerio*
79-20-9	Acetic acid methyl ester	not classified	0.28	300	0.53	*Danio rerio*
79-31-2	2-Methylpropanoic acid	baseline	1.00	147	0.34	--
79-41-4	2-Methylacrylic acid	excess	0.99	85	0.57	*Oncorhynchus mykiss*
79-92-5	Camphene	baseline	4.29	1.9	-0.18	--
80-05-7	Bisphenol A	baseline	3.52	4.6	0.26	*Pimephales promelas*
				11	-0.11	*Cyprinodon variegatus*

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
83-32-9	Acenaphthene	baseline	4.30	1.6	-0.06	*Pimephales promelas*
84-66-2	Diethylphthalate	baseline	2.43	29	0.32	*Cyprinodon variegatus*
				12	0.70	*Oncorhynchus mykiss*
84-74-2	di-n-Butylphthalate	baseline	4.70	0.92	0.12	*Pimephales promelas*
85-68-7	1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester	baseline	4.88	1.16	-0.07	--
86-57-7	1-Nitronaphthalene	not classified	3.09	9	0.19	*Pimephales promelas*
87-56-9	Mucochloric acid	excess	1.03	123	0.67	*Leuciscus idus*
87-60-5	3-Chloro-2-methylaniline	not classified	2.27	33.2	0.19	*Danio rerio*
88-06-2	2,4,6-Trichlorophenol	not classified	3.45	2.26	0.57	--
88-17-5	2-(Trifluoromethyl)-benzenamine	not classified	2.23	30	0.32	*Danio rerio*
88-85-7	Dinoseb	excess	3.68	0.118	1.75	--
89-59-8	4-Chloro-2-nitrotoluene	not classified	3.03	7.9	0.30	*Danio rerio*
89-61-2	1,4-Dichloro-2-nitrobenzene	not classified	3.05	6.3	0.42	*Leuciscus idus*
89-83-8	Thymol	baseline	3.41	3.2	0.33	--
90-30-2	N-Phenyl-1-naphthalenamine	not classified	4.47	0.44	0.52	*Oncorhynchus mykiss*
90-43-7	2-Phenylphenol	baseline	3.14	4	0.50	*Oncorhynchus mykiss*
91-15-6	1,2-Benzenedicarbonitrile	not classified	0.84	22.6	1.44	*Oryzias latipes*
91-22-5	Quinoline	baseline	2.14	46	0.11	*Pimephales promelas*
91-23-6	1-Methoxy-2-nitrobenzene	not classified	1.81	169	-0.12	*Pimephales promelas*
91-68-9	3-(Diethylamino)-phenol	not classified	2.32	17.1	0.50	*Pimephales promelas*
91-94-1	Dichlorobenzidine	not classified	3.36	2.08	0.78	--
92-70-6	3-Hydroxy-2-naphthalenecarboxylic acid	baseline	2.43	61	-0.08	*Danio rerio*
92-88-6	1,1'-Biphenyl-4,4'-diol	baseline	2.80	13	0.29	*Oryzias latipes*
93-58-3	Benzoic acid, methyl ester	not classified	1.83	23	0.68	*Danio rerio*
93-65-2	Mecoprop	baseline	2.94	125	-0.74	--
				240	-1.02	*Oncorhynchus mykiss*
94-09-7	Benzocaine	not classified	1.80	7.2	1.29	*Oncorhynchus mykiss*
94-74-6	(4-Chloro-2-methylphenoxy)-acetic acid	baseline	2.54	91	-0.31	--
94-75-7	(2,4-Dichlorophenoxy)-acetic acid	baseline	2.67	263	-0.84	*Lepomis macrochirus*
95-48-7	2-Methylphenol	baseline	2.06	18	0.50	*Leuciscus idus*
95-49-8	1-Chloro-2-methylbenzene	baseline	3.18	2.3	0.58	*Oncorhynchus mykiss*
95-53-4	o-Toluidine	not classified	1.62	117	0.03	*Leuciscus idus*
				82.5	0.18	*Leuciscus idus*
95-54-5	1,2-Benzenediamine	not classified	-0.003	24	2.01	*Danio rerio*
				44	1.74	*Pimephales promelas*
95-65-8	3,4-Dimethylphenol	baseline	2.61	14	0.23	*Pimephales promelas*
95-79-4	5-Chloro-2-methylbenzenamine	not classified	2.27	16	0.50	*Danio rerio*
95-94-3	1,2,4,5-Tetrachlorobenzene	baseline	4.61	0.3	0.57	*Pimephales promelas*
96-18-4	1,2,3-Trichloropropane	baseline	2.50	49	-0.15	--
96-33-3	2-Propenoic acid methyl ester	excess	0.73	1.1	2.66	*Cyprinodon variegatus*
				3.4	2.17	*Oncorhynchus mykiss*
96-48-0	gamma-Butyrolactone	not classified	-0.44	56	1.88	*Lepomis macrochirus*

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
97-00-7	1-Chloro-2,4-dinitrobenzene	excess	2.27	0.71	2.01	*Danio rerio*
97-02-9	2,4-Dinitrobenzenamine	excess	1.84	2.2	1.82	*Danio rerio*
97-63-2	2-Methyl-2-propenoic acid ethyl ester	not classified	1.51	100	0.21	*Oncorhynchus mykiss*
97-86-9	2-Methyl-2-propenoic acid 2-methylpropyl ester	not classified	2.88	20	-0.08	*Oncorhynchus mykiss*
97-88-1	2-Methyl-2-propenoic acid butyl ester	not classified	2.23	11	0.70	*Pimephales promelas*
				5.57	1.00	*Oryzias latipes*
98-00-0	Furfuryl alcohol	excess	0.45	362	0.43	--
98-06-6	tert-Butylbenzene	baseline	4.00	65	-1.50	*Leuciscus idus*
98-16-8	3-(Trifluoromethyl)-benzenamine	not classified	2.10	35	0.36	*Danio rerio*
98-51-1	Benzene, 1-(1,1-dimethylethyl)-4-methyl-	baseline	4.40	2	-0.26	*Cyprinus carpio*
98-54-4	p-tert-Butylphenol	baseline	3.42	5	0.13	*Oncorhynchus mykiss*
98-94-2	N,N-Dimethylcyclohexylamine	not classified	2.16	31.6	0.25	*Leuciscus idus*
98-95-3	Nitrobenzene	not classified	1.81	92	0.05	*Danio rerio*
99-09-2	3-Nitroaniline	not classified	1.47	153	0.14	*Danio rerio*
99-54-7	3,4-Dichloronitrobenzene	not classified	3.11	5.2	0.46	*Leuciscus idus*
99-71-8	p-sec-Butylphenol	baseline	3.46	0.74	0.92	*Salmo salar*
99-88-7	p-Isopropylaniline	not classified	2.37	42	-0.01	*Danio rerio*
99-91-2	4-Chloroacetophenone	baseline	2.32	33.2	0.19	*Brachidanio rerio*
100-01-6	4-Nitroaniline	not classified	1.47	87.6	0.39	*Danio rerio*
100-37-8	2-(Diethylamino)-ethanol	not classified	0.13	147	1.15	*Leuciscus idus*
100-41-4	Ethylbenzene	baseline	3.03	4.2	0.36	*Oncorhynchus mykiss*
100-42-5	Styrene	baseline	2.90	4.02	0.47	*Pimephales promelas*
100-44-7	Chloromethylbenzene	excess	2.79	4	0.65	*Danio rerio*
				1.9	0.97	*Oryzias latipes*
				5	0.55	*Pimephales promelas*
100-46-9	Benzylamine	not classified	1.04	31.6	1.06	*Leuciscus idus*
100-47-0	Benzonitrile	baseline	1.42	78	0.35	*Lepomis macrochirus*
				32	0.74	*Oncorhynchus mykiss*
100-51-6	Benzyl alcohol	not classified	1.09	10	1.52	*Lepomis macrochirus*
100-52-7	Benzaldehyde	not classified	1.60	1.07	2.09	*Lepomis macrochirus*
				11.2	1.07	*Oncorhynchus mykiss*
				7.5	1.24	--
100-97-0	Urotropine	excess	-4.15	41000	2.16	*Lepomis macrochirus*
101-54-2	N-Phenyl-1,4-benzenediamine	not classified	1.82	1.9	1.90	*Danio rerio*
101-77-9	4,4 -Methylenebis-benzenamine	not classified	1.97	20.6	0.78	*Oryzias latipes*
				39	0.50	*Oncorhynchus mykiss*
101-83-7	Dicyclohexylamine	not classified	4.37	12	-0.92	*Oryzias latipes*
				39	-1.43	*Leuciscus idus*
102-69-2	Tripropylamine	baseline	2.84	38.3	-0.32	*Leuciscus idus*
102-81-8	Dibutylaminoethanol	not classified	3.31	29	-0.48	*Oryzias latipes*
				31.6	-0.52	*Leuciscus idus*
102-82-9	Tributylamine	baseline	4.46	16.3	-1.12	*Oryzias latipes*

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
103-09-3	2-Ethylhexylacetate	baseline	3.97	8.27	-0.47	*Oncorhynchus mykiss*
103-11-7	2-Ethylhexylacrylate	not classified	4.37	46.5	-1.50	--
				1.81	-0.09	*Oncorhynchus mykiss*
103-83-3	Benzyldimethylamine	not classified	1.87	16	0.80	*Leuciscus idus*
103-84-4	Acetanilide	not classified	1.13	100	0.59	*Lepomis macrochirus*
104-76-7	2-Ethyl-1-hexanol	baseline	2.73	17.1	0.08	*Leuciscus idus*
104-78-9	N,N-Diethyl-1,3-propanediamine	not classified	0.45	147	0.95	*Leuciscus idus*
104-90-5	5-Ethyl-2-methyl-pyridine	baseline	2.39	77	-0.34	*Oncorhynchus mykiss*
104-93-8	1-Methoxy-4-methylbenzene	baseline	2.68	68.2	-0.51	*Leuciscus idus*
105-53-3	Diethylmalonate	not classified	0.93	11.8	1.75	*Pimephales promelas*
105-56-6	Cyanoacetic acid ethyl ester	not classified	-0.02	59	1.65	*Danio rerio*
105-59-9	Methyldiethanolamine	not classified	-1.29	1470	1.28	*Leuciscus idus*
105-60-2	Caprolactam	not classified	0.39	707	0.25	*Oncorhynchus mykiss*
105-67-9	2,4-Dimethylphenol	baseline	2.61	16.6	0.15	--
106-37-6	p-Dibromobenzene	baseline	3.77	1.23	0.65	--
106-47-8	p-Chloroaniline	not classified	1.72	23	0.74	*Leuciscus idus*
				13	0.98	*Oncorhynchus mykiss*
				2.5	1.70	*Lepomis macrochirus*
				33	0.58	*Danio rerio*
				13	0.98	*Pimephales promelas*
106-49-0	p-Toluidine	not classified	1.62	160	-0.10	*Danio rerio*
				149	-0.07	*Pimephales promelas*
106-51-4	p-Benzoquinone	not classified	0.25	0.045	4.53	*Pimephales promelas*
				0.125	4.09	*Oncorhynchus mykiss*
106-88-7	1,2-Epoxybutane	excess	0.77	157	0.40	*Leuciscus idus*
106-92-3	(2-Propenyloxy)-methyloxirane	excess	0.45	30	1.57	*Carassius auratus*
107-05-1	3-Chloro-1-propene	excess	1.93	22	0.37	*Pimephales promelas*
107-07-3	2-Chloroethanol	excess	0.03	15.2	2.05	*Gambusia affinis*
107-10-8	1-Propanamine	not classified	0.31	46	1.21	*Leuciscus idus*
107-12-0	Propanenitrile	excess	0.35	340	0.28	*Oncorhynchus mykiss*
				41	1.20	*Lepomis macrochirus*
107-13-1	Propenenitrile	excess	0.21	50	1.21	--
107-15-3	1,2-Ethanediamine	excess	-1.64	640	1.62	*Poecilia reticulata*
				116	2.36	*Pimephales promelas*
107-20-0	Chloroacetaldehyde	excess	0.09	3.35	2.65	*Danio rerio*
107-21-1	1,2-Ethanediol	not classified	-1.28	72900	-0.71	*Pimephales promelas*
107-22-2	Ethanedial	excess	-1.41	570	1.47	*Leuciscus idus*
107-41-5	2,4-Pentanediol, 2-methyl-	baseline	0.58	8510	-0.97	*Gambusia affinis*
				8690	-0.97	*Pimephales promelas*
107-86-8	3-Methyl-2-butenal	excess	0.84	12.7	1.51	*Leuciscus idus*
107-98-2	1-Methoxy-2-propanol	baseline	-0.46	20800	-0.65	*Pimephales promelas*
				7300	-0.19	*Leuciscus idus*

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
				6800	-0.16	*Leuciscus idus*
108-01-0	2-Dimethylaminoethanol	not classified	-0.75	147	1.72	*Leuciscus idus*
108-16-7	1-Dimethylamino-2-propanol	not classified	0.00	148	1.19	*Leuciscus idus*
108-21-4	Isopropylacetate	not classified	1.28	360	-0.21	*Leuciscus idus*
108-31-6	2,5-Furandione	excess	-0.50	75	1.86	*Oncorhynchus mykiss*
108-42-9	m-Chloroaniline	not classified	1.80	18.7	0.76	*Danio rerio*
108-43-0	3-Chlorophenol	baseline	2.16	4.24	1.13	--
108-44-1	m-Toluidine	not classified	1.62	34	0.57	*Oryzias latipes*
108-46-3	1,3-Benzenediol	not classified	1.03	53.4	0.85	*Pimephales promelas*
108-62-3	Metaldehyd	baseline	0.85	150	0.75	--
108-67-8	1,3,5-Trimethylbenzene	baseline	3.53	12.5	-0.45	*Carassius auratus*
108-86-1	Bromobenzene	baseline	2.94	5.6	0.48	*Pimephales promelas*
108-88-3	Toluene	baseline	2.54	5.5	0.57	*Oncorhynchus kisutch*
108-89-4	4-Methylpyridine	baseline	1.29	400	-0.30	*Cyprinodon variegatus*
108-90-7	Chlorobenzene	baseline	2.64	22.2	-0.03	*Poecilia reticulata*
				6.69	0.49	*Oncorhynchus mykiss*
108-91-8	Cyclohexylamine	not classified	1.63	300	-0.42	*Poecilia reticulata*
108-94-1	Cyclohexanone	baseline	1.00	527	-0.17	*Pimephales promelas*
108-95-2	Phenol	baseline	1.51	8.9	1.18	*Oncorhynchus mykiss*
				5	1.43	*Oncorhynchus mykiss*
109-02-4	4-Methylmorpholine	not classified	-0.34	490	0.93	*Leuciscus idus*
109-52-4	Pentanoic acid	baseline	1.68	39	0.44	*Pimephales promelas*
109-55-7	N,N-Dimethyl-1,3-propanediamine	excess	-0.40	122	1.59	*Leuciscus idus*
109-65-9	1-Bromobutane	baseline	2.34	36.7	0.07	*Phoxinus phoxinus*
109-66-0	n-Pentane	baseline	3.02	4.26	0.19	*Oncorhynchus mykiss*
109-67-1	1-Pentene	baseline	2.66	5	0.40	*Oncorhynchus mykiss*
109-73-9	1-Aminobutane	not classified	0.42	32	1.38	*Lepomis macrochirus*
109-76-2	1,3-Propanediamine	excess	-1.09	125	1.98	*Leuciscus idus*
109-77-3	Propanedinitrile	excess	-0.60	0.57	3.89	*Lepomis macrochirus*
				1.6	3.44	*Oncorhynchus mykiss*
109-79-5	1-Butanethiol	excess	2.28	1100	-1.53	*Ictalurus catus*
109-87-5	Dimethoxymethane	baseline	-0.10	6990	-0.54	*Pimephales promelas*
109-89-7	Diethylamine	not classified	0.70	182	0.41	*Oncorhynchus mykiss*
				25	1.27	*Oncorhynchus mykiss*
110-12-3	5-Methyl-2-hexanone	baseline	1.77	159	-0.19	--
110-49-6	2-Methoxyethanol acetate	baseline	0.10	190	1.06	*Carassius auratus*
110-86-1	Pyridine	not classified	0.80	106	0.59	*Pimephales promelas*
110-88-3	1,3,5-Trioxane	baseline	-0.53	4000	0.12	*Leuciscus idus*
110-89-4	Piperidine	not classified	0.93	73	0.68	*Leuciscus idus*
110-91-8	Morpholine	not classified	-0.56	180	1.48	*Oncorhynchus mykiss*
				380	1.15	*Oncorhynchus mykiss*
110-96-3	Diisobutylamine	baseline	2.63	20	0.08	--

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
110-97-4	Diisopropanolamine	not classified	-0.84	1470	0.97	*Danio rerio*
111-26-2	1-Hexanamine	baseline	1.82	14.7	0.75	*Leuciscus idus*
111-29-5	1,5-Pentanediol	baseline	-0.11	4600	-0.21	*Leuciscus idus*
111-30-8	Glutaraldehyde	excess	-0.29	9.4	2.61	*Lepomis macrochirus*
				39	1.99	*Cyprinodon variegatus*
				10.8	2.55	*Pimephales promelas*
111-40-0	Diethylenetriamine	excess	-2.13	430	2.41	*Poecilia reticulata*
111-42-2	2,2 -Iminobis-ethanol	not classified	-1.95	1460	1.74	*Pimephales promelas*
111-44-4	2,2′-Dichlorodiethyl ether	not classified	1.56	600	-0.51	*Lepomis macrochirus*
111-49-9	Hexahydro-1H-azepine	not classified	1.68	57	0.26	*Leuciscus idus*
111-55-7	1,2-Ethanediol, diacetate	not classified	0.40	90	1.24	*Lepomis macrochirus*
111-69-3	Hexanedinitrile	not classified	0.02	670	0.55	*Oncorhynchus mykiss*
111-71-7	Heptanal	not classified	2.55	12	0.32	*Oncorhynchus mykiss*
111-76-2	2-Butoxyethanol	baseline	0.57	1470	-0.20	*Oncorhynchus mykiss*
				1250	-0.12	*Menidia beryllina*
111-77-3	2-(2-Methoxyethoxy)-ethanol	not classified	-0.83	5740	0.32	*Pimephales promelas*
111-87-5	1-Octanol	baseline	2.81	50	-0.45	*Alburnus alburnus*
111-90-0	2-(2-Ethoxyethoxy)-ethanol	baseline	-0.69	12900	-0.09	*Oncorhynchus mykiss*
111-92-2	di-n-Butylamine	baseline	2.42	5.5	0.81	*Oncorhynchus mykiss*
				37	-0.01	*Oncorhynchus mykiss*
112-07-2	2-Butoxyethylacetate	baseline	1.54	28.3	0.89	*Oncorhynchus mykiss*
112-24-3	Triethylenetetramine	excess	-2.32	330	2.83	*Pimephales promelas*
112-25-4	2-(Hexyloxy)-ethanol	baseline	1.76	140	-0.02	*Pimephales promelas*
112-30-1	1-Decanol	baseline	3.79	5	-0.14	*Pimephales promelas*
112-34-5	2-(2-Butoxyethoxy)-ethanol	baseline	0.29	1300	0.22	*Lepomis macrochirus*
112-57-2	Tetraethylenepentamine	excess	-3.16	420	3.50	*Poecilia reticulata*
114-26-1	Propoxur	excess	1.71	6.5	1.51	--
115-18-4	2-Methyl-3-buten-2-ol	excess	0.87	3400	-0.93	*Leuciscus idus*
115-19-5	2-Methyl-3-butyn-2-ol	excess	0.38	3400	-0.56	*Leuciscus idus*
115-86-6	Phosphoric acid, triphenyl ester	excess	4.65	0.4	0.59	*Oncorhynchus mykiss*
117-81-7	Bis(2-ethylhexyl) phthalate	baseline	7.95	9.5	-3.31	*Lepomis macrochirus*
118-48-9	Isatoic acid anhydride	excess	2.15	73	0.00	*Leuciscus idus*
118-74-1	Hexachlorobenzene	not classified	5.86	7.6	-1.71	--
118-92-3	2-Amino-benzoic acid	not classified	1.29	160	0.27	*Leuciscus idus*
119-64-2	1,2,3,4-Tetrahydronaphthalene	baseline	3.87	3.2	-0.09	*Danio rerio*
120-12-7	Anthracene	baseline	4.44	0.0265	1.67	*Lepomis macrochirus*
120-36-5	Dichlorprop	baseline	3.23	2.7	0.74	--
120-61-6	1,4-Benzenedicarboxylic acid, dimethyl ester	not classified	1.66	18.8	1.05	*Danio rerio*
120-82-1	1,2,4-Trichlorobenzene	baseline	3.99	2.4	0.08	*Oryzias latipes*
120-83-2	2,4-Dichlorophenol	baseline	2.90	1.24	1.18	*Carassius auratus*
121-44-8	Triethylamine	baseline	1.51	36	0.61	*Oncorhynchus mykiss*
121-87-9	2-Chloro-4-nitroaniline	not classified	2.12	12	0.83	*Poecilia reticulata*

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
122-14-5	Fenitrothion	excess	3.30	2.2	0.84	--
122-20-3	Triisopropanolamine	not classified	-0.62	3160	0.62	*Leuciscus idus*
122-52-1	Triethyl phosphite	excess	0.74	251	0.59	*Danio rerio*
122-98-5	N-(2-Hydroxyethyl)aniline	not classified	0.65	570	0.22	*Leuciscus idus*
123-05-7	2-Ethylhexanal	not classified	2.71	5.5	0.58	*Oncorhynchus mykiss*
123-31-9	1,4-Benzenediol	not classified	1.03	0.638	2.77	--
123-38-6	Propanal	excess	0.46	14	1.60	*Pimephales promelas*
123-42-2	Diacetonealcohol	baseline	-0.34	420	1.06	*Lepomis macrochirus*
123-54-6	Pentanedione-2,4	excess	0.88	72	0.80	*Oncorhynchus mykiss*
				114	0.60	*Carassius auratus*
				90	0.70	*Pimephales promelas*
123-75-1	Pyrrolidine	not classified	0.46	115	0.78	*Danio rerio*
123-92-2	3-Methyl-1-butanol acetate	baseline	2.26	24	0.30	*Danio rerio*
124-02-7	Diallylamine	baseline	1.31	5	1.60	*Carassius auratus*
124-04-9	Adipic acid	baseline	0.16	230	1.03	*Leuciscus idus*
124-09-4	1,6-Hexanediamine	not classified	0.40	1830	-0.16	*Pimephales promelas*
				62	1.31	*Leuciscus idus*
124-17-4	Butyldiglycol acetate	baseline	1.31	60	0.85	*Danio rerio*
124-40-3	Dimethylamine	excess	-0.22	118	1.11	*Oncorhynchus mykiss*
				17	1.95	*Oncorhynchus mykiss*
125-12-2	Isobornylacetate	baseline	3.86	14	-0.55	*Danio rerio*
126-73-8	Tributylphosphate	excess	3.82	4.5	0.10	*Oryzias latipes*
				8	-0.15	*Oncorhynchus mykiss*
128-39-2	2,6-Di-tert-butylphenol	baseline	4.49	13	-1.00	*Danio rerio*
138-86-3	Limonene	baseline	4.70	80	-2.13	*Oncorhynchus mykiss*
140-11-4	Benzylacetate	baseline	2.02	4	1.33	*Oryzias latipes*
140-29-4	Phenylacetonitril	not classified	1.56	50	0.49	--
140-31-8	N-Aminoethylpiperazine	excess	-1.51	368	2.08	*Leuciscus idus*
140-88-5	Ethylacrylate	excess	1.20	4.6	1.74	*Oncorhynchus mykiss*
141-32-2	Butylacrylate	excess	2.29	2.1	1.33	*Cyprinodon variegatus*
141-43-5	2-Aminoethanol	not classified	-1.76	349	1.98	*Cyprinus carpio*
				170	2.30	*Carassius auratus*
141-78-6	Ethylacetate	not classified	0.86	455	-0.04	*Oncorhynchus mykiss*
142-28-9	1,3-Dichloropropane	baseline	2.16	113	-0.36	--
142-62-1	Hexanoic acid	baseline	1.99	88	-0.10	*Pimephales promelas*
143-07-7	Dodecanoic acid	baseline	4.80	5	-0.84	--
149-30-4	2-Mercaptobenzothiazole	excess	2.64	0.73	1.62	*Oncorhynchus mykiss*
150-78-7	1,4-Dimethoxybenzene	baseline	2.12	127	-0.28	*Danio rerio*
298-07-7	Phosphoric acid, bis(2-ethylhexyl) ester	excess	4.37	30	-1.07	*Oncorhynchus mykiss*
348-54-9	2-Fluoroaniline	not classified	1.43	7.5	1.39	*Danio rerio*
352-32-9	4-Fluorotoluene	baseline	2.66	380	-1.29	*Danio rerio*
357-57-3	2,3-Dimethoxy-strychnidin-10-one	not classified	1.49	28	1.32	--

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
431-03-8	2,3-Butandione	baseline	-1.34	73	2.48	*Leuciscus idus*
503-74-2	3-Methylbutanoic acid	baseline	1.33	500	-0.39	*Leuciscus idus*
504-24-5	4-Pyridinamine	excess	-0.11	4	2.81	--
504-29-0	2-Pyridinamine	not classified	0.53	5.2	2.19	*Lepomis macrochirus*
513-86-0	Acetyl methyl carbinol	excess	-0.36	3400	0.05	*Leuciscus idus*
556-82-1	3-Methyl-2-buten-1-ol	excess	1.04	46.4	0.80	*Leuciscus idus*
586-62-9	Terpinolene	baseline	4.88	1.22	-0.46	*Pimephales promelas*
589-90-2	1,4-Dimethylcyclohexane	baseline	4.01	6.5	-0.58	*Morone saxatilis*
591-27-5	3-Aminophenol	not classified	0.24	0.5	3.50	*Leuciscus idus*
592-46-1	2,4-Hexadiene	baseline	2.86	19.5	-0.28	--
598-56-1	N,N-Dimethylethylamine	baseline	0.57	38.3	1.18	*Leuciscus idus*
611-19-8	1-Chloro-2-(chloromethyl)-benzene	excess	3.44	0.71	0.99	*Danio rerio*
615-65-6	2-Chloro-p-toluidine	not classified	2.27	36.1	0.15	--
616-45-5	2-Pyrrolidinone	not classified	-0.52	7300	-0.18	*Danio rerio*
617-89-0	Furfurylamine	not classified	0.41	10	2.02	*Leuciscus idus*
624-54-4	Propanoic acid, pentyl ester	baseline	2.83	56	-0.47	*Pimephales promelas*
626-67-5	1-Methylpiperidine	not classified	1.28	73	0.48	*Danio rerio*
629-11-8	1,6-Hexanediol	baseline	0.38	7300	-0.74	*Leuciscus idus*
634-66-2	1,2,3,4-Tetrachlorobenzene	baseline	4.44	0.4	0.58	*Poecilia reticulata*
634-67-3	2,3,4-Trichloraniline	not classified	3.01	3.6	0.71	--
634-90-2	1,2,3,5-Tetrachlorobenzene	not classified	4.60	5.05	-0.65	--
636-30-6	2,4,5-Trichloraniline	not classified	3.31	2.37	0.66	*Poecilia reticulata*
645-62-5	2-Ethyl-2-hexenal	not classified	2.50	16	0.27	*Leuciscus idus*
646-06-0	1,2-Dioxolane	baseline	-0.34	10000	-0.51	*Cyprinodon variegatus*
706-31-0	1,5,9-Cyclododecatriene, (E,E,Z)-	baseline	4.79	5.5	-0.96	*Oncrohynchus mykiss*
709-98-8	Propanil	not classified	2.98	6	0.56	--
760-23-6	3,4-Dichloro-1-butene	excess	2.60	8.25	0.48	--
763-32-6	3-Methyl-3-buten-1-ol	baseline	1.07	730	-0.42	*Leuciscus idus*
766-09-6	1-Ethylpiperidine	not classified	1.84	25	0.55	*Leuciscus idus*
929-06-6	2-(2-Aminoethoxy)-ethanol	not classified	-1.55	460	1.93	*Leuciscus idus*
1330-20-7	Dimethylbenzene (mixture)	baseline	3.09	13.5	-0.20	*Oncorhynchus mykiss*
1330-78-5	Phosphoric acid, tris(methylphenyl) ester	excess	6.34	0.6	-0.87	*Oncorhynchus mykiss*
1563-66-2	Carbofuran	excess	2.31	0.48	2.19	--
1570-64-5	4-Chloro-2-methyl-phenol	baseline	2.70	2.3	1.01	*Lepomis macrochirus*
1634-04-4	Methyl-tert-butylether	baseline	1.43	574	-0.59	*Pimephales promelas*
				574	-0.59	*Menidia beryllina*
1663-39-4	t-Butylacrylate	excess	2.21	57	-0.04	--
1738-25-6	3-Dimethylaminopropionitrile	excess	-0.45	730	0.83	*Leuciscus idus*
2243-62-1	1,5-Diaminonaphthalene	not classified	1.12	17.3	1.43	*Danio rerio*
2855-13-2	Isophorondiamine	not classified	1.45	110	0.40	*Leuciscus idus*
				70	0.59	*Danio rerio*
2867-47-2	2-Methyl-2-propenoic acid, 2-(dimethylamino)ethyl ester	excess	1.05	19.1	1.44	*Oryzias latipes*

CAS	Compound	classification	log K_{ow}	LC_{50} [mg/L]	Residuals ($\log 1/LC_{50exp} - \log 1/LC_{50calc}$)	Species
2869-34-3	1-Tridecanamine	baseline	5.25	0.0654	0.69	--
3452-97-9	3,5,5-Trimethyl-1-hexanol	baseline	3.11	27.7	-0.39	*Oryzias latipes*
3724-65-0	2-Butenoic acid	excess	0.85	0.75	2.74	*Danio rerio*
4435-53-4	3-Methoxy-1-butanol, acetate	baseline	1.01	7.1	1.87	*Danio rerio*
5392-40-5	Citral	baseline	3.11	6.8	0.25	*Leuciscus idus*
13360-63-9	n-Ethyl-1-butaneamine	baseline	0.85	26.5	1.26	*Leuciscus idus*
				332	0.17	*Danio rerio*
13952-84-6	2-Butanamine	not classified	0.75	57	0.87	*Leuciscus idus*
17639-93-9	2-Chloro-propanoic acid methyl ester	not classified	1.04	22	1.27	*Leuciscus idus*
24549-06-2	2-Ethyl-6-methylaniline	not classified	2.66	61	-0.41	*Danio rerio*
25321-14-6	2,4-Dinitrotoluolene	excess	2.06	6.3	1.19	*Gasterosteus aculeatus*
25620-58-0	Trimethylhexamethylendiamine	not classified	1.60	10	-0.71	--
26896-18-4	Isononanoic acid	baseline	3.45	160	-1.38	*Oncorhynchus mykiss*
				190	-1.45	*Lepomis macrochirus*
				5	-1.88	*Leuciscus idus*
27458-92-0	Isotridecanol	baseline	5.26	0.42	-0.13	*Oncorhynchus mykiss*
				0.55	-0.25	*Danio rerio*
27458-94-2	Isononanol	baseline	3.22	11	-0.08	*Cyprinus carpio*
84852-15-3	4-Nonylphenol	baseline	5.77	0.138	-0.01	*Pimephales promelas*
				0.19	-0.14	*Oncorhynchus mykiss*

References

1. US EPA, Distributed Structure-Searchable Toxicity (DSSTox) Database, ftp://ftp.epa.gov/dsstoxftp/DSSTox_Archive_20150930/EPAFHM_DownloadFiles/).
2. US EPA, KOWWIN v1.68 from EPISuite, Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11, https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface).
3. M. Nendza and C. L. Russom, *Xenobiotica*, 1991, **21**, 147-170.
4. R. L. Lipnick, *Sci.Tot.Environ.*, 1991, **109/110**, 131-153.
5. R. L. Lipnick, K. R. Watson and A. K. Stausz, *Xenobiotica*, 1987, **17**, 1011-1025.
6. M. Nendza, S. Gabbert, R. Kühne, A. Lombardo, A. Roncaglioni, E. Benfenati, R. Benigni, C. Bossa, S. Strempel, M. Scheringer, A. Fernández, R. Rallo, F. Giralt, S. Dimitrov, O. Mekenyan, F. Bringezu and G. Schüürmann, *Regulatory Toxicology and Pharmacology*, 2013, **66**, 301-314.
7. E. Baum, H. F. Bender, A. Broemme, U. Gundert-Remy, J. Holzhäuser, M. König, M. Nendza, U. Stephan and U. Strobel, *Handbuch der gefährlichen Güter*, Springer, Heidelberg, 2015.
8. M. Hrovat, H. Segner and S. Jeram, *Regulat.Toxicol.*, 2009, **54**, 294-300.