APPENDIX B: DATABASE

Table 4: Fish Acute

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1-Hexanol	111-27-3	OCCCCCC	O	Class 1		-1.239	-3.023
1-Heptanol	111-70-6	OCCCCCCC	O	Class 1		-1.947	-3.485
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1		-2.373	-4.001
1-Nonanol	143-08	OCCCCCCCCC	O	Class 1		-3.052	-4.419
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1		-3.603	-4.838

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1-Undecanol	112-42-5	OCCCCCCCCCCC	O	Class 1		-4.333	-5.236
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-5.270
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.561
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1		-0.444	-2.153
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.371
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.118
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.186
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.643
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.933
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.411
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.817
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.064
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.369
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.202
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.227
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-2.994

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-3.801
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.915
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.667
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.509
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.474
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.521
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.521
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.093
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-3.843
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.296
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.862
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.935
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.924
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-4.879
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.281
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.468

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.207
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.118
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.544
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.099
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.544
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.419
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.845
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.845
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.985
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.969
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.960
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.977
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.451
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.917
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.915
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.958

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.797
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.715
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-4.754
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.403
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-4.080
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.448
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.513
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.377
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.607
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.499
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.666
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.523
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-4.398
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-4.229
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.269
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1		-3.253	-4.177

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.589
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.122
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.116
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.268
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-3.884
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.124
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.257
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.481
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.240
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.763
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.126
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.319
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.812	-3.015
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-3.659
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-3.630
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.268

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-3.535
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 2		0.239	-3.519
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 2		0.239	-2.827
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.021
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.084
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.791
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.792
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.355
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.677
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.922
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.665
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.365
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.086
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.149
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.096
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.303

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.547
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.329
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.280
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.829
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.144
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.135
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.963
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.969
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.290
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.109
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.017
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.804
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.045
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.948
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.310
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.290

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.265
3-Chlorophenol	108-43-0	ClC1=CC(O)=CC=C1	N	Class 2		-0.610	-4.508
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.529
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.180
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.529
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.828
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.361
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.410
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.377
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.696
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.385
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.317
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.944
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.410
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-4.024
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-3.983

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Butyraldehyde	123-72-8	O=CCCC	N	Class 3		-0.159	-3.446
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.416
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.462
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.036
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.462
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.906
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.911
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.416
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-5.763
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	
4-Chlorobenzaldehyde	104-88-1	ClC1=CC=C(C=O)C=C1	N	Class 3		-1.966	-4.805
Benzaldehyde	100-52-7	O=Cc(cccc1)c1	N	Class 3		-1.184	-3.977
Acetaldehyde	75-07-0	O=CC	N	Class 3		1.744	-2.920
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.458
Hexenal	66-25-1	O=CCCCCC	N	Class 3		-1.223	-3.855
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-3.978

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Salicylaldehyde	90-02-8	O=Cc(c(O)ccc1)c1	N	Class 3		-0.856	-4.883
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.001
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.268
Endosulfan	115-29-7	ClC2=C(Cl)C3(Cl)C1COS(=O)OCC1C2(Cl)C3(Cl)Cl	N	Class 4		-5.659	-8.530
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.780
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.773
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.458
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.572
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.703
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.210
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.174
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.342
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-8.095
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.996
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.572

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.233
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.509
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.032
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-8.163
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.851
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.708
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.318
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.589
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.631
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.260
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-4.260
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.121
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-8.233
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.948
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.118
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.896
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.868
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.916
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.294
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.374
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.948

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.169
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.072
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.937
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.374
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.314
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-9.294
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.403
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.050
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.998
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.456

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Fish log L(E)C50 (mol/L)
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.429
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.087
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.001
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.319
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.581
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.662
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.787
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.754
Methyl acetate	79-20-9	O=C(OC)C	N	Class 5		0.516	-2.393
Trifluralin	1582-09-8	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)	N	Class 5		-4.691	-6.571

Table 5: Invertebrate Acute

A = 1.0		**A = 0.1**		**A = 0.01**		**A = 0.001**	
1	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	**CAS #**	**SMILES**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**Updated in this report**	**log S_L (mol/L)**	**Invert log L(E)C50 (mol/L)**
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1		-3.603	-4.737
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-5.384
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.710
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1		-0.444	-3.770
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.672
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.271

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
PBDE	32534-81-9	Brc1cc(c(cc1Oc2c(cc(cc2)Br)Br)Br)Br	O	Class 1			
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-3.498
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.892
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.587
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-2.894
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.179
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.614
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-3.643
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.973
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.739
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.290
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.375
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-3.877
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.791
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.740
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.485

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-5.113
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.088
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.937
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.322
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.126
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.348
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.863
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.827
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-4.256
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.596
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.003
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-4.827
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.083
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-3.365
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-4.250
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.870

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.492
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.492
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-3.636
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-4.427
n-Heptane	142-82-5	CCCCCCCC	O	Class 1		-4.469	-4.825
n-Octane	111-65-9	CCCCCCCCC	O	Class 1		-5.238	-5.581
n-Octane	111-65-11	CCCCCCCCC	O	Class 1		-5.238	-5.581
n-Octane	111-65-12	CCCCCCCCC	O	Class 1		-5.238	-5.478
n-Nonane	111-84-2	CCCCCCCCCC	O	Class 1		-5.766	-5.807
n-Nonane	111-84-3	CCCCCCCCCC	O	Class 1		-5.766	-5.807
2-Methylbutane	78-78-4	CC(C)CC	O	Class 1		-3.179	-4.427
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.971
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.348
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1		-3.253	-4.282
Dec-1-ene	872-05-9	CCCCCCCCC=C	O	Class 1			
Dodec-1-ene	112-41-4	CCCCCCCCCCC=C	O	Class 1			

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.626
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.452
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-3.412
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.334
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-4.969
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-4.646
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.746
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.546
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.659
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-4.405
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.268
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.262
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-4.514
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.317
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.350
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.376

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-5.765
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-5.765
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.248
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.766
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.940
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.371
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-4.482
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-4.905
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-5.154
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-4.899
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.848
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.931
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.812
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.762
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-3.417
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.704

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.397
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.848
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.566
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.033
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.747
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.240
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.694
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.317
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.393
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.711
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.496
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.426
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.277
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.166
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.160
Acetaldehyde	75-07-0	O=CC	N	Class 3		1.744	-2.885

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-4.442
Nonanal	124-19-6	O=CCCCCCCCC	N	Class 3		-3.126	-4.920
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.302
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-6.018
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.900
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.949
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.606
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.856
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.856
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-6.809
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-8.317
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-8.531
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.801
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.606
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.464
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.464

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-9.233
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.464
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-7.765
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.731
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.890
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-7.877
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.508
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.319
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.197
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.271
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.550
DDT	50-29-3	c(ccc(c1)Cl)(c1)C(c(ccc(c2)Cl)c2)C(Cl)(Cl)Cl	N	Class 4		-6.983	-8.152
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-5.921
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.312
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5		-1.665	-3.626
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.239

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log L(E)C50 (mol/L)
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-4.926
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.453
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.280
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.540
Atrazine	1912-24-9	n(c(nc(n1)NC(C)C)NCC)c1Cl	N	Class 5		-2.321	-3.871

Table 6: Algae Acute

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
1-Hexanol	111-27-3	OCCCCCC	O	Class 1		-1.239	-3.106
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1		-2.373	-3.968
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.829
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1		-0.444	-3.535
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.335
Pentanol	94624-12-1	CC(CCC)O	O	Class 1		-0.591	-3.037
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.254
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.042

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-3.953
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-3.886
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-3.557
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-2.466
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-2.876
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.659
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.199
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.775
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-2.667
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-5.113
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-4.503
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-4.511
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.341
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-4.963
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-3.676
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-4.825
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.305
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.055

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.217
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-5.396
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.347
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.710
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.824
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.824
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.895
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-2.824
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.369
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-3.954
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-3.983
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-3.956
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1		-3.253	-4.272
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-3.136
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-4.143
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.842
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.835
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-3.643

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-3.795
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-3.795
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.993
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.010
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.507
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-3.940
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.010
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-4.927
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.359
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-2.726
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-2.094
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-3.188
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-4.139
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-3.984
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.528
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.033
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.867
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.829

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.704
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.168
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.556
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.410
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-3.264
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-2.879
3-Chlorophenol	108-43-0	ClC1=CC(O)=CC=C1	N	Class 2		-0.610	-3.647
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-3.647
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-3.529
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.109
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-4.127
4-Nitrophenol	100-02-7	N(=O)(=O)c(ccc(O)c1)c1	N	Class 2		0.028	-3.638
4-Nitrophenol	100-02-7	N(=O)(=O)c(ccc(O)c1)c1	N	Class 2		0.028	-4.126
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-5.963
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-4.595
4-Chlorobenzaldehyde	104-88-1	ClC1=CC=C(C=O)C=C1	N	Class 3		-1.966	-4.219
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log L(E)C50 (mol/L)
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-5.717
Atrazine	1912-24-9	n(c(nc(n1)NC(C)C)NCC)c1Cl	N	Class 5		-2.321	-6.700

Table 7: Fish Chronic

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-7.552
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.503
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.736
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.608
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.552
1-Methylphenanthrene	832-69-9	c1ccc2c3cccc(C)c3ccc2c1		Class 1		-4.884	-6.284
1,7-Dimethylphenanthrene	483-87-4	Cc3cccc2c3ccc1c2ccc(c1)C		Class 1		-5.488	-7.110
2,7-Dimethylphenanthrene	1576-69-8	c(cc(c1cc2)c(ccc3C)c2c3)c(c1)C		Class 1		-5.488	-7.201
2-Ethylphenanthrene	3674-74-6	c(ccc1c(ccc2CC)c3c2)cc1cc3		Class 1		-5.564	-6.917

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.818
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.459
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.818
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.126
Dibenzothiophene	132-65-0	s(c(c(c1cccc2)ccc3)c3)c12		Class 1		-4.366	-6.265
Retene	483-65-8	c(ccc1c(ccc2C(C)C)c3c2)c(C)c1cc3		Class 1		-6.531	
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-6.066
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-6.029
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.528
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.455
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-5.472
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-6.489
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-5.667
Acenaphthene	83-32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-6.382
Benzo[a]pyrene	50-32-8	c(c(c(cc1)ccc2)c2cc3)(c3cc(c4ccc5)c5)c14		Class 1		-6.767	
Benzo[k]fluoranthene	207-08-9	c2ccc1cc3c(cc1c2)c4cccc5cccc3c45		Class 1		-7.074	-9.040
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-3.010

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Dichloromethane	75-09-2	ClCCl	O	Class 1		-0.815	-2.777
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-4.789
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1		-2.078	-4.359
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.851
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-4.921
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-6.657
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-5.844
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.167
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.866
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.411
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.599
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-3.882
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.754
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.861
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1		-2.028	-4.239
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-4.648
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.866

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.663
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-4.370
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.391
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-4.858
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.836
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-5.234
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-4.247
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1		
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-6.445
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-7.154
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-6.539
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.552
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-5.378
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-4.714
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-6.087
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-5.455
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.704

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.138
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.908
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.908
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-4.507
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-5.604
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.691
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-7.603
Hexachlorobutadiene	87-68-3	Cl/C(Cl)=C(\Cl)C(\Cl)=C(/Cl)Cl	N	Class 3		-5.010	-7.434
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.658
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.867
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.867
Pentachlorobenzene	608-93-5	ClC1=CC(=C(Cl)C(=C1Cl)Cl)Cl	N	Class 4		-4.976	-6.658
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.773
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.875
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.886
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.640
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-8.103
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.792
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.027
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.010
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.195
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.346
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.279
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.195
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.823
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.045
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.457
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.580
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.580
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.753
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.425
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-8.561

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.194
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.319
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-6.963
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-7.493
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-6.289

Table 8: Invertebrate Chronic

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1		-2.373	-5.115
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1		-3.603	-6.158
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-7.124
1-Tetradecanol	112-72-1	OCCCCCCCCCCCCCC	O	Class 1		-5.907	-8.127
1-Pentadecanol	629-76-5	OCCCCCCCCCCCCCCC	O	Class 1		-6.162	-7.467
1-Octadecanol	112-92-5	OCCCCCCCCCCCCCCCCCC	O	Class 1			
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-3.326
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-3.530
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-3.238

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-7.137
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.570
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.495
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.503
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-6.746
Phenanthrene	85-01-8	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3		Class 1		-4.666	-5.996
Perhydrophenanthrene		C(C(C(C(C1)CCC2)C2)CCC3)(C1)C3		Class 1		-6.671	-7.077
Benzene	71-43-2	c(cccc1)c1		Class 1		-1.096	-4.420
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-5.097
Toluene	108-88-3	c(cccc1)(c1)C		Class 1		-2.243	-4.964
Ethylbenzene	100-41-4	c(cccc1)(c1)CC		Class 1		-2.798	-5.046
m-Xylene	108-38-3	c(cccc1C)(c1)C		Class 1		-2.819	-4.905
p-Xylene	106-423	c(ccc(c1)C)(c1)C		Class 1		-2.816	-4.830
Isopropylbenzene	98-82-8	c(cccc1)(c1)C(C)C		Class 1		-3.292	-5.536
1,3,5-Trimethylbenzene	108-67-8	c(cc(cc1C)C)(c1)C		Class 1		-3.397	-5.478
Biphenyl	92-52-2	c(c(cccc1)c1)(cccc2)c2		Class 1		-3.911	-5.958
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.397

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Naphthalene	91-20-3	c(c(ccc1)ccc2)(c1)c2		Class 1		-3.419	-5.330
Acenaphthylene	208-96-8	c1ccc2cccc3c2c1C=C3		Class 1		-3.308	-6.376
Acenaphthene	83--32-9	c(c(ccc1)ccc2)(c1CC3)c23		Class 1		-3.920	-6.565
Fluorene	86-73-7	c(c(c(c1ccc2)c2)ccc3)(c3)C1		Class 1		-4.104	-6.823
Pyrene	129-00-0	c(c(c(cc1)ccc2)c2cc3)(c1ccc4)c34		Class 1		-4.927	-7.984
Benzo[a]pyrene	50-32-8	c(c(c(cc1)ccc2)c2cc3)(c3cc(c4ccc5)c5)c14		Class 1		-6.767	-8.703
Benzo[ghi]perylene	191-24-2	c16cccc2ccc3ccc4ccc5cccc6c5c4c3c12		Class 1		-6.523	-9.528
Indeno(123cd)pyrene	193-39-5	c(c(c(c(ccc1)c2)c1cc3)c3cc4)(c2c(c5ccc6)c6)c45		Class 1			
Dibenz[ah]anthracene	53-70-3	c(c(c(c(c1)ccc2)c2)cc(c3c(c(c4)ccc5)c5)c4)(c1)c3		Class 1		-5.629	-9.967
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-4.278
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1		-2.260	-4.682
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-5.512
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1		-3.044	-5.175
Chlorobutane	109-69-3	ClCCCC	O	Class 1		-2.925	-4.218
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1		-1.098	-3.954
1,2,4-Trichlorobenzene	120-82-1	Clc1ccc(Cl)c(Cl)c1	O	Class 1		-3.681	-6.259
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.328

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.435
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-5.468
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.825
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.690
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.427
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1		-2.975	-5.368
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1		-1.763	-4.386
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.459
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-6.028
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.958
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.870
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.620
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-5.546
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-5.050
Dec-1-ene	872-05-9	CCCCCCCCC=C	O	Class 1		-5.545	-6.859
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.675
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.811

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-5.438
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	Class 1	-2.515	-4.218
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	Class 1	-2.406	-5.292
Dimethyl phthalate	131-11-3	O=C(OC)c(c(ccc1)C(=O)OC)c1		Class 5	Class 1	-1.665	-4.306
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-3.949
Diethyl phthalate	84-66-2	O=C(OCC)c(c(ccc1)C(=O)OCC)c1		Class 5	Class 1	-2.305	-5.365
Dibutyl phthalate	84-74-2	O=C(OCCCC)c(c(ccc1)C(=O)OCCCC)c1	O	Class 5	Class 1	-4.388	-5.462
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.732
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.896
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-5.919
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.942
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2		-2.238	-4.692
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-6.961
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-6.128
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-7.367
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2		0.026	-5.311
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2		-1.650	-7.577

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2		-1.565	-5.406
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.397
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.511
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.210
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.431
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.461
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-7.130
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-6.227
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2		-0.654	-5.410
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-5.310
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.520
Salicylaldehyde	90-02-8	O=Cc(c(O)ccc1)c1	N	Class 3		-0.856	-5.973
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-8.199
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.782
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	-7.756

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Hexachlorobenzene	118-74-1	c1(c(c(c(c(c1Cl)Cl)Cl)Cl)Cl)Cl	N	Class 4		-5.717	
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.948
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.124
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.606
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.332
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.857
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.124
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.170
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.221
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.481
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.425
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.221
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-7.425
Pentachlorophenol	87-86-5	Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl	N	Class 4		-3.474	-6.425
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.396
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.464

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Invert log EC10/NOEC (mol/L)
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.723
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.738
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.080
Butyl benzyl phthalate	85-68-7	O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2		Class 5		-5.063	-6.048
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-8.238
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-7.005
Fluoranthene	206-44-0	c(c(ccc1)ccc2)(c1c(c3ccc4)c4)c23		Class 5		-5.072	-7.075

Table 9: Algae Chronic

A = 1.0		A = 0.1		A = 0.01		A = 0.001	
X	Y	X	Y	X	Y	X	Y
0	0	0	-1	0	-2	0	-3
-1	-1	-1	-2	-1	-3	-1	-4
-2	-2	-2	-3	-2	-4	-2	-5
-3	-3	-3	-4	-3	-5	-3	-6
-4	-4	-4	-5	-4	-6	-4	-7
-5	-5	-5	-6	-5	-7	-5	-8
-6	-6	-6	-7	-6	-8	-6	-9
-7	-7	-7	-8	-7	-9	-7	-10

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log EC10/NOEC (mol/L)
1-Hexanol	111-27-3	OCCCCCC	O	Class 1		-1.239	-3.968
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1		-4.985	-6.668
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1		-5.302	-5.969
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1		-0.432	-2.543
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-3.238
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1		-0.324	-2.273
Ethylbenzene	100-41-4	c(cccc1)(c1)CC		Class 1		-2.798	-4.495
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1		-1.137	-4.521
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1		-3.070	-4.825

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log EC10/NOEC (mol/L)
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1		-2.969	-5.411
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.916
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1		-3.487	-5.897
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1		-1.482	-3.705
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1		-2.351	-4.219
n-Pentane	109-66-0	CCCCCC	O	Class 1		-3.273	-4.557
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1		-3.209	-4.952
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.811	-4.126
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	Class 1	-1.812	-4.161
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	Class 1	-2.497	-4.218
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2		-0.498	-5.604
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.225
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2		-1.594	-5.756
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.106
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2		-0.425	-3.288
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-5.210
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2		-1.986	-4.829
Acetaldehyde	75-07-0	O=CC	N	Class 3		1.744	-2.644

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	Updated in this report	log S_L (mol/L)	Algae log EC10/NOEC (mol/L)
Acrolein	107-02-8	O=CC=C	N	Class 3		0.570	-6.748
Heptanal	111-71-7	O=CCCCCCC	N	Class 3		-1.961	-5.094
Heptachlor	76-44-8	ClC1C=CC2C1C3(Cl)C(=C(Cl)C2(Cl)C3(Cl)Cl)Cl	N	Class 4		-5.619	-7.122
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.066
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-5.233
Lindane	58-89-9	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl	N	Class 4		-3.734	-6.163
Atrazine	1912-24-9	n(c(nc(n1)NC(C)C)NCC)c1Cl	N	Class 5		-2.321	-7.292

Table 10: Polar K_{OW}s and Solubilities

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m^3				OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
3	98-95-3	O	Class 2		123.0	1.9	20	20	1900	20	5.26	15.4471545	ECHA	L	-1.81115151	3596.49123	278.26		1	15.4472	-1.81115151
2-Nitrotoluene	88-72-2	O	Class 2		137.1	2.3	16	20	437	20	-9.3	3.18652472		L	-2.49668271	17434.5283	263.7		1	3.1865	-2.49668271
3-Nitrotoluene	99-08-1		Class 2		137.1	2.4	16	20	419	20	16.1	3.05616338	ECHA	L	-2.51482343	18178.2021	289.1		1	3.0562	-2.51482343
3-Nitrotoluene	99-08-1		Class 2		137.1	2.4	16	20	419	20	16.1	3.05616338	ECHA	L	-2.51482343	18178.2021	289.1		1	3.0562	-2.51482343
4-Nitrotoluene	99-99-0	O	Class 2		137.1	2.4	13	20	345	20	44.5	2.51567741		S	-2.59934505	14161.5327	317.5		0.64126526	3.9230	-2.40638277

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
4-Nitrochlorobenzene	100-00-5	O	Class 2		157.6	2.39	200	20	243	20	83	1.54226961	OECD SIDS dossier 2003	S	-2.8118397	9607.8915	356	Dugal M; Kirk-Othmer, 2005	0.26672326	5.782284	-2.23790059
Bisphenol-A	80-05-7	N	Class 2		228.3	3.4	4.12E-07		301		155	1.31844065	ECHA	S	-2.87993942	2178.97215	428		0.05171122	25.4962	-1.59352418
Aniline	62-53-3	N	Class 2		93.1	0.9	40	20	35000	20	-6.2	375.818748	ECHA	L	-0.42502156	147.825397	266.8		1	375.8187	-0.42502156
Nitroaniline	99-09-2	N	Class 2													#DIV/0!					
Phenol	108-95-2	N	Class 2		94.1	1.5	20	20	70000		40.6	743.810435		S	-0.12853773	52.3474343	313.6		0.70085822	1061.2852	0.02583209

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT										OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
																Vw=	**0.000018**	**mol/m^3**			
4-Nitrophenol	41092.0	N	Class 2													#DIV/0!					
2,4-Dinitrophenol	51-28-5	N	Class 2													#DIV/0!					
4,4'-Methylenedianiline	101-77-9	N	Class 2		198.3	1.6	0.00025		1010		90	5.09329299		S	-2.29300134	2480.39712	363		0.22740101	22.3978	-1.64979372
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	N	Class 2		142.6	3.09	27	20	2300	20	48	16.1301634	Publication 2002	S	-1.79236123	2039.35197	321	Publication 2002	0.59211145	27.241769	-1.56476469
3,4-Dichloroaniline	95-76-1	N	Class 2	Anilines (unhindered)	162.0	2.7	0.294		580	20	71.5	3.58024691	[1]	S	-2.44608702	5378.65493	344.5	Merck Index 2001	0.34662443	10.328894	-1.98594619

[1] European Union Risk Assessment Report: 3,4-dichloroaniline (3,4-DCA), Vol. 65

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT														OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**		**Solubility (mol/m^3)**	**Ref**			**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**Activity Coef (YW)**	**mol/m^3**	**Tm (MP in K)**	**Ref**		**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
2-Chlorophenol	95-57-8	N	Class 2		128.55	2.15	139		28500	20	9.3		221.703617	Chlor Euro Marine 2002	RA		L	-0.65422722			250.584795		282.3	Chlor Euro Marine 2002	RA	1	221.703617	-0.65422722
3-Chlorophenol	108-43-0	N	Class 2		128.55	2.50	125		26000	20	33.5		202.255932	Chlor Euro Marine 2019	RA		S	-0.69409873			226.315585		306.5	Chlor Euro Marine 2019	RA	0.82392605	245.478258	-0.60998697
4-Chlorophenol	106-48-9	N	Class 2		128.55	2.39	51		27100	20	43		210.812913	Chlor Euro Marine 2025	RA		S	-0.67610279			174.868366		316	Chlor Euro Marine 2025	RA	0.66356118	317.699288	-0.49798376
MoA 1																												

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m³				OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m³)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m³)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
1-Hexanol	111-27-3	O	Class 1		102.2				5900	20	-47.5	57.7299413		L	-1.23859888	962.335217	225.5		1	57.7299	-1.23859888
1-Heptanol	111-70-6	O	Class 1		116.2				1313	20	-34	11.2994836		L	-1.9469414	4916.64551	239		1	11.2995	-1.9469414
1-Octanol	111-87-5	O	Class 1		130.2				551		-16.25	4.23195084		L	-2.37345939	13127.6467	256.75		1	4.2320	-2.37345939
1-Nonanol	143-08	O	Class 1		144.3				128	20	-5	0.88704089		L	-3.05205636	62630.2083	268		1	0.8870	-3.05205636
1-Decanol	112-30-1	O	Class 1		158.3				39.5		6.4	0.24952622		L	-3.60288382	222644.163	279.4		1	0.2495	-3.60288382

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
1-Undecanol	112-42-5	O	Class 1		172.3				8	20	14.3	0.04643064		L	-4.33319529	1196527.78	287.3		1	0.0464	-4.33319529
1-Dodecanol	112-53-8	O	Class 1		186.3				1.93	20	23.3	0.01035963		L	-4.98465555	5362694.3	296.3		1	0.0104	-4.98465555
1-Tridecanol	112-70-9	O	Class 1		200.4				0.38	20	30.6	0.00189621		S	-5.72211412	25788543	303.6		0.88020775	0.0022	-5.66669931
1-Tetradecanol	112-72-1	O	Class 1		214.4				0.191		39.5	0.00089086		S	-6.05019141	44816107.5	312.5		0.71864635	0.0012	-5.90670664
1-Pentadecanol	629-76-5	O	Class 1		228.4				0.102		44	0.00044658		S	-6.35009593	80687988.5	317		0.64861273	0.0007	-6.16208139

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
1-Hexadecanol	36653-82-4	O	Class 1		242.4				0.013		50	5.363E-05		S	-7.27058926	586042636	323		0.56573423	0.0001	-7.02320172
1-Octadecanol	112-92-5	O	Class 1		270.5	7.4			0.0011		58	4.0665E-06		S	-8.39077458	6440958786	331		0.4714639	0.0000	-8.06422303
Isotridecanol	27458-92-0	O	Class 1		200.37	5.19			1	20	-78	0.00499077		L	-5.3018327	11131666.7	195		1	0.0050	-5.3018327
Cyclohexanol	108-93-0	O	Class 1		100.16	1.25			36000	20	24	359.42492		L	-0.4439182	154.567901	297		1	359.4249	-0.4439182
Benzyl alcohol	100-51-6	O	Class 1		108.14	1.05			40000	20	-15.4	369.890882		L	-0.43192637	150.194444	257.6		1	369.8909	-0.43192637

Vw= **0.000018** **mol/m^3**

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT				Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Pentanol	94624-12-1	O	Class 1		88.15	1.29, 1.51, 1.35			22600		-138	256.381168		L	-0.59111388	216.691249	135		1	256.3812	-0.59111388
tert-Butyl methyl ether	1634-04-4	O	Class 1		88.2	1.1	33000		41850	20	-108	474.758934	ECHA	L	-0.32352685	117.018452	165		1	474.7589	-0.32352685
PBDE	32534-81-9	O	Class 1		564.7	6.5	very low!		0.0024	20	-7	4.2503E-06		L	-8.37157578	1.3071E+10	266		1	0.0000	-8.37157578
Phenanthrene	85-01-8		Class 1		178.2	4.4			1.15		78	0.00645197		S	-5.19030733	2573790.74	351		0.2989086	0.0216	-4.66584574
1-Methylphenanthrene	832-69-9		Class 1		192.3	5.1			0.269		123	0.00139915		S	-5.85413666	4257013.01	396		0.10721136	0.0131	-4.88437748

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT				Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
1,7-Dimethylphenanthrene	483-87-4		Class 1		206.3	5.4			0.099		108.94	0.00047991		S	-6.31884298	17097871.8	381.94		0.14769697	0.0032	-5.48821456
2,7-Dimethylphenanthrene	1576-69-8		Class 1		206.3	5.4			0.099		108.94	0.00047991		S	-6.31884298	17097871.8	381.94		0.14769697	0.0032	-5.48821456
2-Ethylphenanthrene	3674-74-6		Class 1		206.3	5.4			0.096		102.68	0.00046536		S	-6.33220694	20335359.7	375.68		0.17034031	0.0027	-5.56352436
Perhydrophenanthrene			Class 1		192.4	5.2			0.041		20.83	0.00021315		L	-6.67130833	260636856	293.83		1	0.0002	-6.67130833
Benzene	71-43-2		Class 1		78.11	2.1			1790		80	22.9163999		S	-1.63985361	692.354475	353		0.2855929	80.2415	-1.09560101

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT				Vw=	0.000018	mol/m^3				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m^3)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m^3)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Ethylbenzene	100-41-4		Class 1		106.2	3.2			169		-94.9	1.59178676		L	-2.79811511	34901.3807	178.1		1	1.5918	-2.79811511
m-Xylene	108-38-3		Class 1		106.2	3.2			161		-47.8	1.5164359		L	-2.81917594	36635.6108	225.2		1	1.5164	-2.81917594
p-Xylene	106-423		Class 1		106.2	3.1			162		13.2	1.52585476		L	-2.8164868	36409.465	286.2		1	1.5259	-2.8164868
Isopropylbenzene	98-82-8		Class 1		120.2	3.7			61.3		-96	0.50998336		L	-3.29244399	108936.016	177		1	0.5100	-3.29244399
1,3,5-Trimethylbenzene	108-67-8		Class 1		120.2	3.4			48.2		-44.7	0.40099834		L	-3.39685743	138543.107	228.3		1	0.4010	-3.39685743

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Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{ow}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
Biphenyl	92-52-2		Class 1		154.2	4.0			6.94		69	0.04500357		S	-4.34675307	452979.432	342		0.36694242	0.1226	-3.91135099
Dibenzothiophene	132-65-0		Class 1		184.3	4.2			1.47		99	0.00797786		S	-5.09811373	1289953.62	372		0.18523919	0.0431	-4.3658466
Dimethyl DBT	1207-12-1		Class 1		212.3	5.3			0.09		117	0.00042391		S	-6.37272794	16109025.6	390		0.12291753	0.0034	-5.46234178
Dimethyl phenanthrene	1576-67-6		Class 1		206.3	5.4			0.07133		109	0.00034578		S	-6.46120595	23697978.3	382		0.14749519	0.0023	-5.6299838
Retene	483-65-8		Class 1		234.3	6.4			0.00848		117	3.6187E-05		S	-7.44145057	188708692	390		0.12291753	0.0003	-6.53106441

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Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**				**log S_L (mol/L)**
																Activity Coef (YW)	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**		
Retene	483-65-8		Class 1		234.3	6.4			0.00848		117	3.6187E-05		S	-7.44145057	188708692	390		0.12291753	0.0003		-6.53106441
7,12-DMBA	57-97-6		Class 1		256.4	6.6			0.061		154	0.00023796		S	-6.62350349	12351259.6	427		0.052903	0.0045		-5.34698376
Naphthalene	91-20-3		Class 1		128.2	3.2			31		45	0.2418474		S	-3.61645857	145638.445	318		0.63400103	0.3815		-3.41854854
Acenaphthylene	208-96-8		Class 1		152.2	3.9			16.1		92.5	0.10578187		S	-3.97558878	112815.793	365.5		0.21480957	0.4924		-3.30764241
Fluorene	86-73-7		Class 1		166.2	4.2			1.69		114.8	0.01016725		S	-4.99279657	706167.958	387.8		0.12923613	0.0787		-4.10418051

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Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
Pyrene	129-00-0		Class 1		202.3	4.9			0.135		151.2	0.00066746		S	-6.17557623	4693441.44	424.2		0.05638813	0.0118	-4.92676391
Pyrene	129-00-0		Class 1		202.3	4.9			0.135		151.2	0.00066746		S	-6.17557623	4693441.44	424.2		0.05638813	0.0118	-4.92676391
Benz[a]anthracene	56-55-3		Class 1		228.3	5.8			0.0094		84	4.1174E-05		S	-7.38537806	351779840	357		0.26071463	0.0002	-6.80154345
Benzo[a]pyrene	50-32-8		Class 1		252.3	6.1			0.00162		6.4204E-06	6.4204E-06		S	-8.19243666	325245951	442		0.03758787	0.0002	-6.7674844
Benzo[ghi]perylene	191-24-2		Class 1		276.3	6.6			0.00026		278	9.4087E-07		S	-9.02647041	185197853	551		0.00313645	0.0003	-6.52290845

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Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Benzo[k]fluoranthene	207-08-9		Class 1		252.32	6.11			0.0008		169	3.1706E-06		S	-8.49886169	658623052	442		0.03758787	0.0001	-7.07390943
Indeno(123cd)pyrene	193-39-5		Class 1		276.3	6.7			0.00019		163.6	6.8756E-07		S	-9.16269015	3434797196	436.6		0.04250925	0.0000	-7.7911736
Dibenz[ah]anthracene	53-70-3		Class 1		278.4	6.8			0.00249		269.5	8.9453E-06		S	-8.04840748	23642031.4	542.5		0.00380671	0.0023	-5.62895729
Dichloromethane	75-09-2	O	Class 1		84.926	1.25	58400	20	13000	25	-95	153.074441	Horvath AL; Halogenated Hydrocarbons: Solubility-Miscibility With Water NY: Marcel Dekker (1982)	L	-0.81509732	362.931624	178	CRC handbook of chemistry and physics. 66th ed. Boca	1	153.074441	-0.81509732
Chloroform	67-66-3	O	Class 1		119.368	1.97	21100	20	8700	23	-63.5	72.883855	Study, 1995	L	-1.13736866	762.247765	209.5	Merck Index 1976	1	72.883855	-1.13736866

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Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**		**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**		**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
Carbon tetrachloride	56-23-5	O	Class 1		153.81	2.83	12000	20	846		-23		5.50029257	Study, 2010	L	-2.25961421					10100.4728	250	Dreisbach, R. R.;Martin, R. A., Ind. Eng. Chem., 41 (12),	1	5.500293	-2.25961421
Trichloroethylene	79-01-6	O	Class 1		131.5	2.53	9900	20	1100	20	-85		8.36501901	Mackay D, Shiu WY, Ma KC, 1993	L	-2.07753307					6641.41414	188	Merck Index 1989	1	8.365019	-2.07753307
Tetrachlorethylene	127-18-4	O	Class 1		165.9	2.53	2500		150		-22		0.90415913	CRC Handbook, 1994	L	-3.04375513					61444.4444	251	Merck Index 1989	1	0.904159	-3.04375513
Chlorobutane	109-69-3	O	Class 1		92.6	2.66	12060	20	110	20	-123		1.18841832	Study report, 2010	L	-2.92503066					46747.4747	150	Review article 1929	1	1.188418	-2.92503066
1,2-Dichloroethane	107-06-2	O	Class 1		99.0	1.45	10247		7900		-36		79.8366885	Banerjee, S.; Yalkowsky, S.H.; Valvani, *S. C. Environ. Sci. Technol.* 14, 1227 - 1229. 1980	L	-1.09779749					695.864979	237	Nabert, K., Schoen, G. (1963). Sicherheitstechnische Kenn zahlen brennbarer Gase und Daempfe, 2. Aufl., Deutscher Eichverlag GmbH, Braunschweig, 68.	1	79.836688	-1.09779749

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Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**		**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
1,2,4-Trichlorobenzene	120-82-1	O	Class 1		181.5	4.05	26	20	37.8		17	0.20826446	Lide DR (ed.) CRC Handbook of Chemistry and Physics (82nd) 2001-2002	L	-3.68138483	**Activity Coef (YW)**	266754.85	**Tm (MP in K)**	290	Ullmann's Encyclopedia of Industrial Chemistry, Wiley-VCH Verlag GmbH & Co. KGaA, 2006	1	0.208264	-3.68138483
1,3-Dichlorobenzene	541-73-1	O	Class 1		147.0	3.44	188	20	125		-24.76	0.85034014	HSDB handbook 2009	L	-3.07040732		65333.3333		248.24	Merck Index 2006	1	0.850340	-3.07040732
1,4-Dichlorobenzene	106-46-7	O	Class 1		147.0	3.37	53		82.9		53.3	0.56394558	Lide DR (ed.) CRC Handbook of Chemistry and Physics (82nd) 2001-2002	S	-3.2487628		51694.888		326.3	Merck Index 2001	0.52475586	1.074682	-2.9687201
1,2-Dichlorobenzene	95-50-1	O	Class 1		147.0	3.38	208	20	155.8		-17.03	1.05986395	Banerjee S. 1984. Environ Sci. Technol. 16: 624-627	L	-2.97474988		52417.6294		255.97	Merck Index 2001	1	1.059864	-2.97474988
1,1,2,2-Tetrachloroethane	79-34-5	O	Class 1		167.9	2.39	650	20	2900	20	-44	17.277331	WHO CICAD3	L	-1.76252335		3215.51724		229		1	17.277331	-1.76252335

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT											OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Vw=**	**0.000018**	**mol/m^3**		**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
1,2,3-Trichlorobenzene	87-61-6	O	Class 1		181.5	4.139	27.93		30.9		53.5	0.17029485	CRC Handbook of Chemistry and Physics, 82 ed.	S	-3.76879849	**Activity Coef (YW)**	170413.575	**Tm (MP in K)**	326.5	**Ref**	CRC Handbook of Chemistry and Physics, 76 ed.	0.52236997	0.326004	-3.48677669
1,1,1-Trichloroethane	71-55-6	O	Class 1		133.4	2.46	15500	20	1250	23	-33	9.37031484	Broholm K; Feenstra S, 1995	L	-2.02824582		5928.88889		240		ATSDR Toxicological profile for 1,1,1-	1	9.370315	-2.02824582
1,1,2-Trichloroethane	79-00-5	O	Class 1		133.4	1.89	2300	20	4400	20	-36	32.9835082	Handbook	L	-1.48170315		1684.34343		237		Merck Index 1986	1	32.983508	-1.48170315
Chlorobenzene	108-90-7	O	Class 1		112.6	2.84	11700	20	502	20	-46	4.45984364	Banerjee S *et al* 1984. Environ Sci Technol 18:587-591	L	-2.35068037		12456.8393		227		Thieme Römpp Online 2008	1	4.459844	-2.35068037
n-Pentane	109-66-0	O	Class 1		72.15	3.45	68400		38.5	20	-106.92	0.53361053	ESR RAR 2003	L	-3.27277561		104112.554		166.08			1	0.533611	-3.27277561

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m^3				OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{ow}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
n-Hexane	110-54-3	O	Class 1		86.18	4.11	20200		9.5		-93.84	0.11023439	EHC Monograph 122, 1991	L	-3.95768288	503976.608	179.16		1	0.110234	-3.95768288
n-Heptane	142-82-5	O	Class 1		100.2	4.64	6110		3.4		-90.6	0.03393214	PhysProp Database	L	-4.4693888	1637254.9	182.4		1	0.033932	-4.4693888
n-Octane	111-65-9	O	Class 1		114.23	5.15	1800		0.66		-56.8	0.00577782	PhysProp Database	L	-5.23823624	9615319.87	216.2		1	0.005778	-5.23823624
n-Nonane	111-84-2	O	Class 1		128.26	5.65	571		0.22		-53.5	0.00171527	TPHC Vol 3	L	-5.76566855	32388888.9	219.5		1	0.001715	-5.76566855
n-Decane	124-18-5	O	Class 1		142.28	6.25	175		0.052		-29.7	0.00036548	PhysProp Database	L	-6.43714051	152008547	243.3		1	0.000365	-6.43714051

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m^3				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m^3)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m^3)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
n-Undecane	1120-21-4	O	Class 1		156.31	6.86	52.2		0.0044		-25.6	2.8149E-05	PhysProp Database	L	-7.55053409	1973611111	247.4		1	0.000028	-7.55053409
n-Dodecane	112-40-3	O	Class 1		170.34	7.41	15.4		0.0037		-9.6	2.1721E-05	PhysProp Database	L	-7.66311492	2557657658	263.4		1	0.000022	-7.66311492
n-Tridecane	629-50-5	O	Class 1		184.36	7.96	4.6		5.56E-04		-5.3	3.02E-06	ETC, 24, 9, 2382 (2005)	L	-8.52059191	1.8421E+10	267.7		1	0.000003	-8.52059191
2-Methylbutane	78-78-4	O	Class 1		72.15	2.72	91800		47.8		-159.9	6.63E-01	OECD SIDS C5 Aliphatics (McAuliffe 1966)	L	-3.17880844	83856.3459	113.1		1	0.662509	-3.17880844
Cyclopentane	287-92-3	O	Class 1		70.134	2.76	36230		156		-93.9	2.22431346	ECHA Database	L	-2.65280401	24976.4957	179.1		1	2.224313	-2.65280401

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT					Vw=	0.000018	mol/m³				OUTPUT
Substance name	CAS #	WoE Narc/non-narc (O/N)	Verhaar Modified	ECOSA 1.11 Class	mol wt (g/mol)	log K_{OW}	Vapour pressure (Pa)	At T°C (if not 25)	Water sol (g/m³)	At T°C (if not 25)	Tm (°C)	Solubility (mol/m³)	Ref	Solid or Liquid at 25°C (S/L)	log S_L (mol/L)	Activity Coef (YW)	Tm (MP in K)	Ref	Fugacity ratio (F)	SS to S_L conversion	log S_L (mol/L)
Cyclohexane	110-82-7	O	Class 1		84.1608	3.38	12400		52		6.5	0.61786485	ECHA Database	L	-3.20910651	89915.3846	279.5		1	0.617865	-3.20910651
Hex-1-ene	592-41-6	O	Class 1		84.16	3.39	24800		47	20	-139.8	0.55846008	ECHA Database	L	-3.25300787	99479.9054	133.2		1	0.558460	-3.25300787
Dec-1-ene	872-05-9	O	Class 1		140.27	5.62	210		0.4		-66.3	0.00285164	ETC, 24, 9, 2382 (2005)	L	-5.54490481	19481944.4	206.7		1	0.002852	-5.54490481
Dodec-1-ene	112-41-4	O	Class 1		168.32	6.7	20		0.032		-35.2	0.00019011	ETC, 24, 9, 2382 (2005)	L	-6.72098574	292222222	237.8		1	0.000190	-6.72098574
Tetradec-1-ene	1120-36-1	O	Class 1		196.38	7.08	1.65		0.0135		-12	6.8744E-05	ECHA Database	L	-7.16276349	808148148	261		1	0.000069	-7.16276349

	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT	INPUT				Vw=	0.000018	mol/m^3				OUTPUT
Substance name	**CAS #**	**WoE Narc/non-narc (O/N)**	**Verhaar Modified**	**ECOSA 1.11 Class**	**mol wt (g/mol)**	**log K_{OW}**	**Vapour pressure (Pa)**	**At T°C (if not 25)**	**Water sol (g/m^3)**	**At T°C (if not 25)**	**Tm (°C)**	**Solubility (mol/m^3)**	**Ref**	**Solid or Liquid at 25°C (S/L)**	**log S_L (mol/L)**	**Activity Coef (YW)**	**Tm (MP in K)**	**Ref**	**Fugacity ratio (F)**	**SS to S_L conversion**	**log S_L (mol/L)**
2-Ethoxyethyl acetate	111-15-9	N	Class 1		132.2	0.6	326		229000	20	-61	1732.74818		L	0.23873545	32.0621058	212		1	1732.7482	0.23873545

Table 11: K_{OW} v LC50

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1-Hexanol	111-27-3	OCCCCCC	O	Class 1	-1.239	-3.023	
1-Heptanol	111-70-6	OCCCCCCC	O	Class 1	-1.947	-3.485	
1-Octanol	111-87-5	OCCCCCCCC	O	Class 1	-2.373	-4.001	
1-Nonanol	143-08	OCCCCCCCCC	O	Class 1	-3.052	-4.419	
1-Decanol	112-30-1	OCCCCCCCCCC	O	Class 1	-3.603	-4.838	
1-Undecanol	112-42-5	OCCCCCCCCCCC	O	Class 1	-4.333	-5.236	
1-Dodecanol	112-53-8	OCCCCCCCCCCCC	O	Class 1	-4.985	-5.270	
Isotridecanol	27458-92-0	OCCCCCCCCCCC(C)C	O	Class 1	-5.302	-5.561	5.19
Cyclohexanol	108-93-0	OC(CCCC1)C1	O	Class 1	-0.444	-2.153	1.25
Benzyl alcohol	100-51-6	OCc(cccc1)c1	O	Class 1	-0.432	-2.371	1.05
Pentanol	94624-12-1	CC(CCC)O	O	Class 1	-0.591	-3.174	1.35
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1	-0.324	-2.118	1.1
tert-Butyl methyl ether	1634-04-4	O(C(C)(C)C)C	O	Class 1	-0.324	-2.186	1.1
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.643	1.25

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.933	1.25
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.228	1.25
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.411	1.25
Dichloromethane	75-09-2	ClCCl	O	Class 1	-0.815	-2.587	1.25
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.817	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.064	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.369	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.202	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-3.227	1.97
Chloroform	67-66-3	ClC(Cl)Cl	O	Class 1	-1.137	-2.994	1.97
Carbon tetrachloride	56-23-5	ClC(Cl)(Cl)Cl	O	Class 1	-2.260	-3.801	2.83
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.915	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.667	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.380	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.403	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.509	2.53

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.474	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.294	2.53
Trichloroethylene	79-01-6	ClC=C(Cl)Cl	O	Class 1	-2.078	-3.341	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.521	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.521	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.093	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.106	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.311	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.757	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.843	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-4.296	2.53
Tetrachlorethylene	127-18-4	Cl/C(Cl)=C(/Cl)Cl	O	Class 1	-3.044	-3.955	2.53
Chlorobutane	109-69-3	ClCCCC	O	Class 1	-2.925	-3.113	2.66
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.862	1.45
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.362	1.45
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.935	1.45

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1,2-Dichloroethane	107-06-2	ClCCCl	O	Class 1	-1.098	-2.924	1.45
1,2,4-Trichlorobenzene	120-82-1	CLC1CCC(CL)C(CL)C1	O	Class 1	-3.681	-4.879	4.05
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1	-3.070	-4.281	3.44
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1	-3.070	-4.468	3.44
1,3-Dichlorobenzene	541-73-1	C1=CC(=CC(=C1)Cl)Cl	O	Class 1	-3.070	-4.207	3.44
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-5.118	3.44
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-5.074	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-5.031	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.611	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.015	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.099	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.955	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.544	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.419	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.298	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.845	3.37

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.514	3.37
1,4-Dichlorobenzene	106-46-7	ClC1=CC=C(Cl)C=C1	O	Class 1	-2.969	-4.845	3.37
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.985	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.969	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.960	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.977	3.38
1,2-Dichlorobenzene	95-50-1	c1ccc(c(c1)Cl)Cl	O	Class 1	-2.975	-4.451	3.38
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.917	2.39
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.915	2.39
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.958	2.39
1,1,2,2-Tetrachloroethane	79-34-5	ClC(Cl)C(Cl)Cl	O	Class 1	-1.763	-3.797	2.39
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1	-3.487	-5.715	4.139
1,2,3-Trichlorobenzene	87-61-6	C1=CC(=C(C(=C1)Cl)Cl)Cl	O	Class 1	-3.487	-4.754	4.139
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.404	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-4.080	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.448	2.46

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.513	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.268	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.274	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.377	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.607	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-2.955	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.499	2.46
1,1,1-Trichloroethane	71-55-6	C(Cl)(Cl)(Cl)C	O	Class 1	-2.028	-3.666	2.46
1,1,2-Trichloroethane	79-00-5	ClCC(Cl)Cl	O	Class 1	-1.482	-3.523	1.89
Chlorobenzene	108-90-7	c1ccc(cc1)Cl	O	Class 1	-2.351	-4.398	2.84
n-Pentane	109-66-0	CCCCCC	O	Class 1	-3.273	-4.229	3.45
Cyclohexane	110-82-7	C(CCCC1)C1	O	Class 1	-3.209	-4.269	3.38
Hex-1-ene	592-41-6	CCCCC=C	O	Class 1	-3.253	-4.177	3.39
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 1	0.239	-3.519	0.6
2-Ethoxyethyl acetate	111-15-9	O=C(OCCOCC)C	N	Class 1	0.239	-2.827	0.6
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	-1.811	-3.126	1.9

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	-1.811	-3.319	1.9
Nitrobenzene	98-95-3	N(=O)(=O)c(cccc1)c1	O	Class 2	-1.812	-3.015	1.9
2-Nitrotoluene	88-72-2	N(=O)(=O)c(c(ccc1)C)c1	O	Class 2	-2.497	-3.387	2.3
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	-2.515	-3.630	2.4
3-Nitrotoluene	99-08-1	N(=O)(=O)c(cccc1C)c1		Class 2	-2.515	-4.268	2.4
4-Nitrotoluene	99-99-0	N(=O)(=O)c(ccc(c1)C)c1	O	Class 2	-2.406	-3.305	2.4
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2	-2.238	-4.021	2.39
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2	-2.238	-4.084	2.39
4-Nitrochlorobenzene	100-00-5	[O-][N+](=O)C1=CC=C(Cl)C=C1	O	Class 2	-2.238	-3.791	2.39
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2	-1.565	-4.792	3.09
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2	-1.565	-4.355	3.09
4-Chloro-o-cresol (4-Chloro-2-methyl phenol)	1570-64-5	CC1=C(C=CC(=C1)Cl)O	N	Class 2	-1.565	-4.677	3.09
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.922	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.665	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.365	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.086	2.7

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.149	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.096	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.303	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.547	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.329	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.280	2.7
3,4-Dichloroaniline	95-76-1	C1=CC(=C(C=C1N)Cl)Cl	N	Class 2	-1.986	-4.829	2.7
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.144	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.135	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.963	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.969	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.290	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.109	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.017	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.804	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.045	2.15

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-3.948	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.310	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.290	2.15
2-Chlorophenol	95-57-8	ClC1=C(O)C=CC=C1	N	Class 2	-0.654	-4.265	2.15
3-Chlorophenol	108-43-0	ClC1=CC(O)=CC=C1	N	Class 2	-0.610	-4.508	2.50
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.529	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.180	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.529	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.828	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.361	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.410	2.39
4-Chlorophenol	106-48-9	OC1=CC=C(Cl)C=C1	N	Class 2	-0.498	-4.377	2.39
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2	-1.594	-4.696	2.39
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2	-1.594	-4.385	3.4
Bisphenol-A	80-05-7	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1	N	Class 2	-1.594	-4.317	3.4
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2	-0.425	-3.944	0.9

Substance name	CAS #	SMILES	WoE Narc/non-narc (O/N)	Verhaar Modified	log S_L (mol/L)	Fish log L(E)C50 (mol/L)	log K_{OW}
Aniline	62-53-3	Nc(cccc1)c1	N	Class 2	-0.425	-3.410	0.9
Phenol	108-95-2	Oc(cccc1)c1	N	Class 2	0.026	-4.024	1.5
4,4'-Methylenedianiline	101-77-9	Nc(ccc(c1)Cc(ccc(N)c2)c2)c1	N	Class 2	-1.650	-3.983	1.6