

Molecule name	logKoa exp	logKoa calc	Diff
(3-(2,3-Epoxypropoxy)propyl)trimethoxysilane	5.8	6.4	-0.60
(Bromomethyl)benzene	4.65	4.85	-0.20
(Chloromethyl)benzene	3.74	4.51	-0.77
(E) 2-Ethylhexyl 4-methoxycinnamate	9.7	8.88	0.82
(Trichloromethyl)benzene	4.15	5.42	-1.27
(Z)-2-Ethylhexyl 4-methoxycinnamate	9.08	8.88	0.20
1-(3-Methylphenyl)ethanone	5.6	5.22	0.38
1,1,1,2-Tetrachloroethane	3.89	3.79	0.10
1,1,1-Trifluoro-2-(2,2,2-trifluoroethoxy)ethane	1.88	2.39	-0.51
1,1,1-Trifluoro-2-propanol	3.62	3.53	0.09
1,1,1-Trifluoroacetone	3.51	2.41	1.10
1,1,2,2-Tetrachloroethane	4.26	3.82	0.44
1,1,2-Trichloroethane	3.54	3.35	0.19
1,10-Decyl dinitrate	8.75	8.14	0.61
1,16-Hexadecanolide	7.31	7.49	-0.18
1,1-Dichloro-2-fluoroethane	1.87	1.87	0.00
1,1-Dichloroethane	2.41	2.57	-0.16
1,1-Dichloropropane	2.81	3	-0.19
1,1-Dichloropropene	2.51	2.87	-0.36
1,1-Diethoxyethane	3.14	3.86	-0.72
1,1-Difluoroethane	0.85	1.21	-0.36
1,1'-Dimethyl-3,3',4,4'-tetrabromo-5,5'-dichloro-2,2'-bipyrrole	13.04	12.6	0.44
1,1'-Dimethyl-3,3',4-tribromo-4',5,5'-trichloro-2,2'-bipyrrole	11.6	12.21	-0.61
1,1'-Dimethyl-3,4,4'-tribromo-3',5,5'-trichloro-2,2'-bipyrrole	12.41	12.21	0.20
1,1-Dimethyl-3-phenylurea	7.85	8.54	-0.69
1,2,3,4,5,6,7-Heptachloronaphthalene	10.63	9.92	0.71
1,2,3,4,5,6,8-Heptachloronaphthalene	10.68	9.92	0.76
1,2,3,4,5,6-Hexachloronaphthalene	10.11	9.32	0.79
1,2,3,4,5,7-Hexachloronaphthalene	9.8	9.32	0.48
1,2,3,4,5,8-Hexachloronaphthalene	10.37	9.32	1.05
1,2,3,4,5-Pentabromo-6-ethylbenzene	9.26	8.81	0.45
1,2,3,4,5-Pentachloronaphthalene	9.28	8.72	0.56
1,2,3,4,6,7,8-Heptachlorodibenzofuran	11.17	11.34	-0.17
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	11.42	11.38	0.04
1,2,3,4,6,7-Hexachloronaphthalene	9.69	9.32	0.37
1,2,3,4,6,8,9-Heptachlorodibenzofuran	11.17	11.34	-0.17
1,2,3,4,6,8-Hexachlorodibenzofuran	10.44	10.74	-0.30
1,2,3,4,6-Pentachloronaphthalene	8.9	8.72	0.18
1,2,3,4,7,8,9-Heptachlorodibenzofuran	11.43	11.34	0.09
1,2,3,4,7,8-Hexachlorodibenzofuran	10.77	10.74	0.03

1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	11.11	10.78	0.33
1,2,3,4,7-Pentachlorodibenzofuran	10.12	10.14	-0.02
1,2,3,4,7-Pentachlorodibenzo-p-dioxin	10.67	10.18	0.49
1,2,3,4,8,9-Hexachlorodibenzofuran	10.95	10.74	0.21
1,2,3,4-Tetrachlorobenzene	5.83	5.72	0.11
1,2,3,4-Tetrachlorodibenzofuran	9.47	9.54	-0.07
1,2,3,4-Tetrachlorodibenzo-p-dioxin	9.7	9.58	0.12
1,2,3,4-Tetrachloronaphthalene	8.33	8.12	0.21
1,2,3,4-Tetrahydronaphthalene	4.65	5.37	-0.72
1,2,3,5,6,7-Hexachloronaphthalene	9.69	9.32	0.37
1,2,3,5,6,8-Hexachloronaphthalene	9.8	9.32	0.48
1,2,3,5,7,8-Hexachloronaphthalene	9.82	9.32	0.50
1,2,3,5,7-Pentachloronaphthalene	8.72	8.72	0.00
1,2,3,5,8-Pentachloronaphthalene	9.1	8.72	0.38
1,2,3,5-Tetrachlorobenzene	5.78	5.72	0.06
1,2,3,5-Tetrachloronaphthalene	8.26	8.12	0.14
1,2,3,6,7,8-Hexachlorodibenzofuran	10.78	10.74	0.04
1,2,3,6,7,8-Hexachlorodibenzo-p-dioxin	10.97	10.78	0.19
1,2,3,6,7-Pentachloronaphthalene	9.1	8.72	0.38
1,2,3,6,8-Pentachloronaphthalene	9.16	8.72	0.44
1,2,3,7,8,9-Hexachlorodibenzofuran	10.93	10.74	0.19
1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	11.01	10.78	0.23
1,2,3,7,8-Pentachlorodibenzofuran	10.43	10.14	0.29
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	10.57	10.18	0.39
1,2,3,7-Tetrachlorodibenzofuran	9.42	9.54	-0.12
1,2,3,7-Tetrachlorodibenzo-p-dioxin	9.94	9.58	0.36
1,2,3,7-Tetrachloronaphthalene	8.35	8.12	0.23
1,2,3,8,9-Pentachlorodibenzofuran	10.48	10.14	0.34
1,2,3,8-Tetrachloronaphthalene	8.6	8.12	0.48
1,2,3-Propanetriol	7.63	7.68	-0.05
1,2,3-Trichlorobenzene	5.16	5.12	0.04
1,2,3-Trichloronaphthalene	7.62	7.52	0.10
1,2,3-Trichloropropane	4.15	4.09	0.06
1,2,4,5,6,8-Hexachloronaphthalene	9.69	9.32	0.37
1,2,4,5,6-Pentachloronaphthalene	9.15	8.72	0.43
1,2,4,5,7,8-Hexachloronaphthalene	9.89	9.32	0.57
1,2,4,5,7-Pentachloronaphthalene	8.86	8.72	0.14
1,2,4,5,8-Pentachloronaphthalene	9.18	8.72	0.46
1,2,4,5-Tetrachlorobenzene	5.8	5.72	0.08
1,2,4,5-Tetrachloronaphthalene	8.58	8.12	0.46
1,2,4,5-Tetramethylbenzene	5.08	4.66	0.42
1,2,4,6,7,8-Hexachlorodibenzofuran	10.5	10.74	-0.24

1,2,4,6,7,9-Hexachlorodibenzo-p-dioxin	10.93	10.78	0.15
1,2,4,6,7-Pentachloronaphthalene	8.73	8.72	0.01
1,2,4,6,8,9-Hexachlorodibenzofuran	10.55	10.74	-0.19
1,2,4,6,8-Pentachloronaphthalene	8.78	8.72	0.06
1,2,4,6-Tetrachloronaphthalene	8.08	8.12	-0.04
1,2,4,7,8-Pentachlorodibenzofuran	9.96	10.14	-0.18
1,2,4,7,8-Pentachlorodibenzo-p-dioxin	10.24	10.18	0.06
1,2,4,7,8-Pentachloronaphthalene	9.06	8.72	0.34
1,2,4,7-Tetrachloronaphthalene	8.13	8.12	0.01
1,2,4,8-Tetrachloronaphthalene	8.41	8.12	0.29
1,2,4-Trichlorobenzene	5.1	5.12	-0.02
1,2,4-Trichlorodibenzo-p-dioxin	8.97	8.98	-0.01
1,2,4-Trichloronaphthalene	7.27	7.52	-0.25
1,2,4-Trimethylbenzene	4.2	4.28	-0.08
1,2,5,6-Tetrabromocyclooctane	7.4	7.54	-0.14
1,2,5,6-Tetrachloronaphthalene	8.22	8.12	0.10
1,2,5,6-Tetramethylnaphthalene	7.33	6.94	0.39
1,2,5,7-Tetrachloronaphthalene	8.08	8.12	-0.04
1,2,5,8-Tetrachloronaphthalene	8.4	8.12	0.28
1,2,5-Trichloronaphthalene	7.45	7.52	-0.07
1,2,6,7-Tetrachloronaphthalene	8.34	8.12	0.22
1,2,6-Trichloronaphthalene	7.5	7.52	-0.02
1,2,7,8-Tetrachlorodibenzofuran	9.78	9.54	0.24
1,2,7,8-Tetrachlorodibenzo-p-dioxin	9.96	9.58	0.38
1,2,7,8-Tetrachloronaphthalene	8.65	8.12	0.53
1,2,7-Trichloronaphthalene	7.54	7.52	0.02
1,2,9,10-Tetrachlorodecane	7.28	7.88	-0.60
1,2-Benzenedicarboxylic acid, di-2-propenyl ester	7.92	7.9	0.02
1,2-Butanediol	6.02	6.03	-0.01
1,2-Butyl dinitrate	5.01	5.31	-0.30
1,2-Decyl dinitrate	7.84	7.89	-0.05
1,2-Dibromobenzene	5.2	5.18	0.02
1,2-Dibromoethane	3.69	3.56	0.13
1,2-Dibutoxyethane	5.22	5.14	0.08
1,2-Dichlorobenzene	4.39	4.52	-0.13
1,2-Dichloronaphthalene	6.83	6.92	-0.09
1,2-Dichloropropane	2.96	3.31	-0.35
1,2-Difluorobenzene	2.86	2.96	-0.10
1,2-Dihydroxybenzene	7.69	8.02	-0.33
1,2-Dimethylbenzene	3.92	3.9	0.02
1,2-Dimethylnaphthalene	6.31	6.18	0.13
1,2-Diphenylethane	7.01	6.58	0.43

1,2-Ethanediol	5.34	5.42	-0.08
1,2-Ethanediol dinitrate	4.55	4.7	-0.15
1,2-Hexyl dinitrate	5.88	6.17	-0.29
1,2-Octyl dinitrate	6.83	7.03	-0.20
1,2-Pentyl dinitrate	5.42	5.74	-0.32
1,2-Propanediol	5.48	5.6	-0.12
1,2-Propyl dinitrate	4.64	4.88	-0.24
1,3,5,7-Tetrachloronaphthalene	7.9	8.12	-0.22
1,3,5,8-Tetrachloronaphthalene	8.26	8.12	0.14
1,3,5-Cycloheptatriene	3.38	3.72	-0.34
1,3,5-Tribromo-2-(2,3-dibromopropoxy)benzene	8.77	9.36	-0.59
1,3,5-Tribromo-2-prop-2-enoxybenzene	6.8	7.15	-0.35
1,3,5-Tribromobenzene	6.1	6.11	-0.01
1,3,5-Trichlorobenzene	4.91	5.12	-0.21
1,3,5-Trichloronaphthalene	7.32	7.52	-0.20
1,3,5-Trichlorotrifluorobenzene	4.71	4.58	0.13
1,3,5-Trimethylbenzene	4.18	4.28	-0.10
1,3,5-Trinitrobenzene	7.83	7.58	0.25
1,3,5-Trioxane	2.55	2.63	-0.08
1,3,6,8-Tetrachlorodibenzofuran	9.75	9.54	0.21
1,3,6,8-Tetrachlorodibenzo-p-dioxin	9.38	9.58	-0.20
1,3,6,8-Tetrachloronaphthalene	8.22	8.12	0.10
1,3,7,8-Tetrachlorodibenzofuran	9.32	9.54	-0.22
1,3,7,8-Tetrachlorodibenzo-p-dioxin	9.86	9.58	0.28
1,3,7,9-Tetrachlorodibenzofuran	9.82	9.54	0.28
1,3,7,9-Tetrachlorodibenzo-p-dioxin	9.93	9.58	0.35
1,3,7-Trichlorodibenzo-p-dioxin	9.63	8.98	0.65
1,3,7-Trimethylnaphthalene	6.61	6.56	0.05
1,3-Butyl dinitrate	5.21	5.31	-0.10
1,3-Butyleneglycol	6.01	6.03	-0.02
1,3-Diaminobenzene	6.64	7.44	-0.80
1,3-Dibromobenzene	5.1	5.18	-0.08
1,3-Dibromopropane	3.79	3.99	-0.20
1,3-Dichloro-2-propanol	4.31	5.08	-0.77
1,3-Dichlorobenzene	4.29	4.52	-0.23
1,3-Dichlorofluoranthene	10.11	10.7	-0.59
1,3-Dichloropropane	3.53	3.31	0.22
1,3-Diethylbenzene	5.18	4.7	0.48
1,3-Difluorobenzene	2.71	2.96	-0.25
1,3-Dihydroxybenzene	9.24	8.02	1.22
1,3-Dimethylbenzene	3.81	3.9	-0.09
1,3-Dimethylnaphthalene	6.31	6.18	0.13

1,3-Dinitrobenzene	6.28	6.16	0.12
1,3-Dioxolane	2.41	2.57	-0.16
1,3-Propanediol	5.59	5.85	-0.26
1,4,5,8-Tetrachloronaphthalene	8.45	8.12	0.33
1,4,5-Trichloronaphthalene	7.56	7.52	0.04
1,4,5-Trimethylnaphthalene	7.04	6.56	0.48
1,4,6,7-Tetrachloronaphthalene	8.13	8.12	0.01
1,4,6,7-Tetramethylnaphthalene	7.16	6.94	0.22
1,4,6-Trichloronaphthalene	7.27	7.52	-0.25
1,4,6-Trimethylnaphthalene	6.66	6.56	0.10
1,4-Benzoquinone	4.68	4.98	-0.30
1,4-Butyl dinitrate	5.66	5.56	0.10
1,4-Cyclohexadiene	2.71	3.5	-0.79
1,4-Diaminoanthraquinone	10.85	10.36	0.49
1,4-Dibromobenzene	5.21	5.18	0.03
1,4-Dibromobutane	4.48	4.42	0.06
1,4-Dichlorobenzene	4.3	4.52	-0.22
1,4-Dichloronaphthalene	6.92	6.92	0.00
1,4-Diethylbenzene	4.75	4.7	0.05
1,4-Difluorobenzene	2.93	2.96	-0.03
1,4-Dihydroxybenzene	9.03	8.02	1.01
1,4-Dimethylbenzene	3.79	3.9	-0.11
1,4-Dimethylnaphthalene	6.51	6.18	0.33
1,4-Dinitrobenzene	6.28	6.16	0.12
1,4-Dinitrobutane	4.61	4.88	-0.27
1,4-Dioxane	3.17	2.9	0.27
1,4-Pentadiene	1.87	2.04	-0.17
1,4-Pentyl dinitrate	5.8	5.74	0.06
1,5-Dichloronaphthalene	6.65	6.92	-0.27
1,5-Dichloropentane	4.47	4.17	0.30
1,5-Dimethylnaphthalene	6.3	6.18	0.12
1,5-Hexadiene	2.21	2.44	-0.23
1,5-Hexyl dinitrate	6.04	6.17	-0.13
1,5-Pentenediol	7.38	6.71	0.67
1,5-Pentyl dinitrate	6.02	5.99	0.03
1,6,7-Trichloronaphthalene	7.54	7.52	0.02
1,6-Dimethylnaphthalene	6.22	6.18	0.04
1,6-Hexanedioic acid	10.74	10.62	0.12
1,6-Hexyl dinitrate	6.69	6.42	0.27
1,7-Dimethylnaphthalene	6.49	6.18	0.31
1,7-Heptyl dinitrate	7.23	6.85	0.38
1,8-Cineole	4.87	4.67	0.20

1,8-Dichlorooctane	5.92	5.46	0.46
1,8-Dimethylnaphthalene	6.56	6.18	0.38
1,8-Octyl dinitrate	7.71	7.28	0.43
12-Oxahehexadecanolide	7.74	7.25	0.49
1-Aminoanthraquinone	10.28	9.81	0.47
1-Bromo-3-chloropropane	3.72	3.65	0.07
1-Bromo-3-fluorobenzene	3.8	4.07	-0.27
1-Bromo-4-chlorobenzene	4.81	4.85	-0.04
1-Bromo-4-fluorobenzene	4.11	4.07	0.04
1-Bromobutane	3.08	3.3	-0.22
1-Bromodecane	5.99	5.88	0.11
1-Bromonaphthalene	6.03	6.65	-0.62
1-Bromooctane	4.72	5.02	-0.30
1-Bromopentane	3.51	3.73	-0.22
1-Bromopropane	2.53	2.87	-0.34
1-Bromopyrene	10.1	10.83	-0.73
1-Butanol	4.1	4.2	-0.10
1-Butene	1.5	1.85	-0.35
1-Butylamine	3.61	3.98	-0.37
1-Butyne	1.59	1.92	-0.33
1-Chloro-1,1-difluoroethane	1.27	1.37	-0.10
1-Chloro-2,4-dinitrobenzene	7.02	6.76	0.26
1-Chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene	9.74	9.6	0.14
1-Chloro-2-[2,2-dichloro-1-(4-chlorophenyl)vinyl]benzene	9.26	9.28	-0.02
1-Chloro-3-fluorobenzene	3.4	3.74	-0.34
1-Chlorobutane	2.72	2.96	-0.24
1-Chlorodibenzo-p-dioxin	7.86	7.78	0.08
1-Chloroheptane	4.07	4.25	-0.18
1-Chlorohexane	3.76	3.82	-0.06
1-Chloronaphthalene	5.81	6.32	-0.51
1-Chlorooctane	4.55	4.68	-0.13
1-Chloropentane	3.19	3.39	-0.20
1-Chloropropane	2.24	2.53	-0.29
1-Chloropyrene	9.71	10.5	-0.79
1-Decene	4.47	4.25	0.22
1-Dodecanol	7.78	7.64	0.14
1-Ethoxy-butane	3.16	3.23	-0.07
1-Ethyl naphthalene	6.2	6.2	0.00
1H-Benzotriazole	5.99	5.91	0.08
1-Heptanol	5.51	5.49	0.02
1-Heptene	2.93	3.05	-0.12
1-Heptyne	2.97	3.12	-0.15

1-Hexadecanol	9.9	9.36	0.54
1-Hexanol	5.18	5.06	0.12
1-Hexene	2.41	2.65	-0.24
1-Hexyne	2.58	2.72	-0.14
1-Hydroxyanthraquinone	9.87	10.1	-0.23
1-Iodobutane	3.33	3.38	-0.05
1-Iodoheptane	4.68	4.67	0.01
1-Iodopentane	3.81	3.81	0.00
1-Methyl-4-isopropyl-7-oxabicyclo[2.2.1]heptane	5.06	4.78	0.28
1-Methyl-4-isopropylcyclohexene	4.04	4.33	-0.29
1-Methylfluorene	7.75	7.52	0.23
1-Methylnaphthalene	5.57	5.8	-0.23
1-Methylphenanthrene	7.89	8.08	-0.19
1-Naphthaleneacetic acid	9.33	9.75	-0.42
1-Naphthylamine	7.42	7.78	-0.36
1-Nitrobutane	3.67	3.53	0.14
1-Nitronaphthalene	7.24	7.14	0.10
1-Nitrooxy-2-butanol	5.83	5.64	0.19
1-Nitrooxy-2-propanol	5.62	5.21	0.41
1-Nitropentane	4.03	3.96	0.07
1-Nitropropane	3.25	3.1	0.15
1-Nonanol	6.5	6.35	0.15
1-Nonene	3.83	3.85	-0.02
1-Nonyne	3.93	3.92	0.01
1-Octadecanol	10.93	10.22	0.71
1-Octanol	6.03	5.92	0.11
1-Octen-3-ol	5.13	5.46	-0.33
1-Octyne	3.53	3.52	0.01
1-Pentanol	4.69	4.63	0.06
1-Pentene	1.93	2.25	-0.32
1-Pentyl nitrate	3.03	4.3	-1.27
1-Pentyne	2	2.32	-0.32
1-Phenyl-1-propanone	5.46	5.24	0.22
1-Propanol	3.68	3.77	-0.09
1-Propylamine	3.6	3.55	0.05
1-Tridecanol	8.19	8.07	0.12
1-Undecanol	7.27	7.21	0.06
2-(3,4-Epoxy cyclohexyl)ethyltriethoxysilane	8.45	7.88	0.57
2-(4-Bromophenoxy)phenol	8.3	9.46	-1.16
2,2,2-Trichloroethanol	5.15	5.03	0.12
2,2,2-Trifluoroethanol	3.33	3.35	-0.02
2,2,3,3,3-Pentafluoro-1-propanol	3.69	3.58	0.11

2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	11.47	11.54	-0.07
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	11.31	10.94	0.37
2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	10.93	11.54	-0.61
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	10.82	10.94	-0.12
2,2',3,3',4,4',5,6-Octachlorobiphenyl	11.12	10.94	0.18
2,2',3,3',4,4',5-Heptachlorobiphenyl	10.78	10.34	0.44
2,2',3,3',4,4',6,6'-Octachlorobiphenyl	10.22	10.94	-0.72
2,2',3,3',4,4',6-Heptachlorobiphenyl	10.25	10.34	-0.09
2,2',3,3',4,4'-Hexachlorobiphenyl	10.36	9.74	0.62
2,2',3,3',4,4'-Hexachlorodiphenyl ether	9.55	9.78	-0.23
2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	10.93	11.54	-0.61
2,2',3,3',4,5,5',6'-Octachlorobiphenyl	10.67	10.94	-0.27
2,2',3,3',4,5,5',6-Octachlorobiphenyl	10.73	10.94	-0.21
2,2',3,3',4,5,5'-Heptachlorobiphenyl	10.38	10.34	0.04
2,2',3,3',4,5,6,6'-Octachlorobiphenyl	10.74	10.94	-0.20
2,2',3,3',4,5',6,6'-Octachlorobiphenyl	10.51	10.94	-0.43
2,2',3,3',4,5',6-Heptachlorobiphenyl	9.88	10.34	-0.46
2,2',3,3',4,5,6'-Heptachlorobiphenyl	10.22	10.34	-0.12
2,2',3,3',4,5',6'-Heptachlorobiphenyl	10.29	10.34	-0.05
2,2',3,3',4,5,6-Heptachlorobiphenyl	10.3	10.34	-0.04
2,2',3,3',4,5'-Hexachlorobiphenyl	9.3	9.74	-0.44
2,2',3,3',4,5-Hexachlorobiphenyl	10.07	9.74	0.33
2,2',3,3',4,6,6'-Heptachlorobiphenyl	9.8	10.34	-0.54
2,2',3,3',4,6'-Hexachlorobiphenyl	9.8	9.74	0.06
2,2',3,3',4,6-Hexachlorobiphenyl	9.49	9.74	-0.25
2,2',3,3',4-Pentabromodiphenyl ether	11.14	10.83	0.31
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	10.08	10.94	-0.86
2,2',3,3',5,5',6-Heptachlorobiphenyl	9.83	10.34	-0.51
2,2',3,3',5,6,6'-Heptachlorobiphenyl	9.81	10.34	-0.53
2,2',3,3',5,6'-Hexachlorobiphenyl	9.42	9.74	-0.32
2,2',3,3',5,6-Hexachlorobiphenyl	9.44	9.74	-0.30
2,2',3,3',5-Pentachlorobiphenyl	9.13	9.14	-0.01
2,2',3,3',6,6'-Hexachlorobiphenyl	9.27	9.74	-0.47
2,2',3,3',6-Pentachlorobiphenyl	8.8	9.14	-0.34
2,2',3,3'-Tetrachlorobiphenyl	8.86	8.54	0.32
2,2',3,4,4',5,5',6-Octachlorobiphenyl	10.79	10.94	-0.15
2,2',3,4,4',5,5'-Heptachlorobiphenyl	10.52	10.34	0.18
2,2',3,4,4',5,5'-Heptachlorodiphenyl ether	9.15	10.38	-1.23
2,2',3,4,4',5,6-Heptachlorobiphenyl	10.51	10.34	0.17
2,2',3,4,4',5',6-Heptachlorobiphenyl	10.32	10.34	-0.02
2,2',3,4,4',5'-Hexachlorobiphenyl	9.81	9.74	0.07
2,2',3,4,4',5-Hexachlorobiphenyl	10.1	9.74	0.36

2,2',3,4,4',5'-Hexachlorodiphenyl ether	9.45	9.78	-0.33
2,2',3,4,4',5'-Hexachlorodiphenyl ether	9.14	9.78	-0.64
2,2',3,4,4',6'-Hexachlorobiphenyl	9.62	9.74	-0.12
2,2',3,4,4',6'-Hexachlorodiphenyl ether	9.04	9.78	-0.74
2,2',3,4,4'-Pentabromodiphenyl ether	11.63	10.83	0.80
2,2',3,4,4'-Pentachlorobiphenyl	9.52	9.14	0.38
2,2',3,4,4'-Pentachlorodiphenyl ether	8.71	9.18	-0.47
2,2',3,4,5,5',6'-Heptachlorobiphenyl	10.4	10.34	0.06
2,2',3,4,5,5',6'-Heptachlorobiphenyl	10.27	10.34	-0.07
2,2',3,4,5,5'-Hexachlorobiphenyl	9.79	9.74	0.05
2,2',3,4,5,5'-Hexachlorobiphenyl	9.56	9.74	-0.18
2,2',3,4,5,6'-Hexachlorobiphenyl	9.39	9.74	-0.35
2,2',3,4,5,6'-Hexachlorobiphenyl	9.34	9.74	-0.40
2,2',3,4,5,6'-Hexachlorobiphenyl	9.47	9.74	-0.27
2,2',3,4,5'-Pentachlorobiphenyl	9.21	9.14	0.07
2,2',3,4,5'-Pentachlorobiphenyl	9.18	9.14	0.04
2,2',3,4,6'-Pentachlorobiphenyl	8.94	9.14	-0.20
2,2',3,4'-Tetrachlorobiphenyl	8.64	8.54	0.10
2,2',3,4'-Tetrachlorobiphenyl	8.58	8.54	0.04
2,2',3,5,5',6'-Hexachlorobiphenyl	9.61	9.74	-0.13
2,2',3,5',6'-Pentachlorobiphenyl	8.8	9.14	-0.34
2,2',3,5'-Tetrachlorobiphenyl	8.36	8.54	-0.18
2,2',3,6,6'-Pentachlorobiphenyl	8.53	9.14	-0.61
2,2',3,6'-Tetrachlorobiphenyl	8.32	8.54	-0.22
2,2',3,6'-Tetrachlorobiphenyl	8.62	8.54	0.08
2,2',3-Trichlorobiphenyl	7.76	7.94	-0.18
2,2',4,4',5,5'-Hexabromobiphenyl	12	11.72	0.28
2,2',4,4',5,5'-Hexabromodiphenyl ether	12.15	11.76	0.39
2,2',4,4',5,5'-Hexachlorobiphenyl	9.8	9.74	0.06
2,2',4,4',5,5'-Hexachlorodiphenyl ether	8.64	9.78	-1.14
2,2',4,4',5,6'-Hexabromodiphenyl ether	11.94	11.76	0.18
2,2',4,4',5,6'-Hexachlorodiphenyl ether	8.41	9.78	-1.37
2,2',4,4',5-Pentabromodiphenyl ether	11.45	10.83	0.62
2,2',4,4',5-Pentachlorobiphenyl	9.24	9.14	0.10
2,2',4,4',5-Pentachlorodiphenyl ether	8.39	9.18	-0.79
2,2',4,4',6,6'-Hexachlorobiphenyl	8.99	9.74	-0.75
2,2',4,4',6-Pentabromodiphenyl ether	11.18	10.83	0.35
2,2',4,4',6-Pentachlorodiphenyl ether	8.14	9.18	-1.04
2,2',4,4'-Tetrabromodiphenyl ether	10.34	9.9	0.44
2,2',4,4'-Tetrachlorobiphenyl	8.31	8.54	-0.23
2,2',4,4'-Tetrachlorodiphenyl ether	8.08	8.58	-0.50
2,2',4,5,5'-PCB	9.04	9.14	-0.10

2,2',4,5,5'-Pentachlorodiphenyl ether	8.14	9.18	-1.04
2,2',4,5',6-Pentabromobiphenyl	10.46	10.79	-0.33
2,2',4,5'-Tetrabromobiphenyl	9.83	9.86	-0.03
2,2',4,5'-Tetrachlorobiphenyl	8.3	8.54	-0.24
2,2',4,5-Tetrachlorobiphenyl	8.25	8.54	-0.29
2,2',4,6,6'-Pentachlorobiphenyl	8.16	9.14	-0.98
2,2',4,6'-Tetrachlorobiphenyl	7.95	8.54	-0.59
2,2',4-Tribromodiphenyl ether	9.27	8.97	0.30
2,2',4-Trichlorobiphenyl	7.51	7.94	-0.43
2,2',4-Trichlorodiphenylether	8.09	7.98	0.11
2,2',5,5'-Tetrachlorobiphenyl	8.25	8.54	-0.29
2,2',5,6'-Tetrachlorobiphenyl	7.93	8.54	-0.61
2,2',5-Trichlorobiphenyl	7.56	7.94	-0.38
2,2',6,6'-Tetrachlorobiphenyl	7.76	8.54	-0.78
2,2',6-Trichlorobiphenyl	7.54	7.94	-0.40
2,2-Dichloro-1,1,1-trifluoroethane	1.78	2.58	-0.80
2,2'-Dichlorobiphenyl	6.86	7.34	-0.48
2,2'-Dichlorodiisopropyl ether	4.3	4.29	0.01
2,2-Dichloropropane	2.3	2.56	-0.26
2,2-Dichloropropionic acid	6.53	5.75	0.78
2,2-Dimethyl-1,3-dioxolane	3.38	3.59	-0.21
2,2-Dimethylpropane	1.41	1.66	-0.25
2,3,3',4,4',5,5',6-Octachlorobiphenyl	11.31	10.94	0.37
2,3,3',4,4',5,5'-Heptachlorobiphenyl	11.22	10.34	0.88
2,3,3',4,4',5,6-Heptachlorobiphenyl	10.57	10.34	0.23
2,3,3',4,4',5',6-Heptachlorobiphenyl	10.62	10.34	0.28
2,3,3',4,4',5-Hexabromodiphenyl ether	11.98	11.76	0.22
2,3,3',4,4',5'-Hexachlorobiphenyl	10.77	9.74	1.03
2,3,3',4,4',5-Hexachlorobiphenyl	10.57	9.74	0.83
2,3,3',4,4',6-Hexachlorobiphenyl	9.86	9.74	0.12
2,3,3',4,4'-Pentachlorobiphenyl	9.53	9.14	0.39
2,3,3',4,4'-Pentachlorodiphenyl ether	8.89	9.18	-0.29
2,3,3',4',5,5',6-Heptachlorobiphenyl	10.53	10.34	0.19
2,3,3',4,5,5'-Hexachlorobiphenyl	9.91	9.74	0.17
2,3,3',4,5,6-Hexachlorobiphenyl	10.32	9.74	0.58
2,3,3',4',5,6-Hexachlorobiphenyl	9.89	9.74	0.15
2,3,3',4',6-Pentachlorobiphenyl	9.06	9.14	-0.08
2,3,3',4'-Tetrachlorobiphenyl	8.45	8.54	-0.09
2,3,3',4-Tetrachlorobiphenyl	8.81	8.54	0.27
2,3,3',5,5',6-Hexachlorobiphenyl	10.36	9.74	0.62
2,3,3'-Trichlorobiphenyl	8.24	7.94	0.30
2,3',4,4',5,5'-Hexachlorodiphenyl ether	8.93	9.78	-0.85

2,3,4,4',5,6-Hexachlorobiphenyl	10	9.74	0.26
2,3,4,4',5-Pentachlorobiphenyl	10.04	9.14	0.90
2,3',4,4',5-Pentachlorobiphenyl	9.47	9.14	0.33
2,3',4,4',6-Pentabromodiphenyl ether	11.52	10.83	0.69
2,3',4,4',6-Pentachlorobiphenyl	9.03	9.14	-0.11
2,3',4,4'-Tetrabromodiphenyl ether	10.58	9.9	0.68
2,3,4,4'-Tetrachlorobiphenyl	9.13	8.54	0.59
2,3',4,4'-Tetrachlorobiphenyl	9.02	8.54	0.48
2,3',4,4'-Tetrachlorodiphenyl ether	8.22	8.58	-0.36
2,3,4,5,6-Pentachlorobiphenyl	9.06	9.14	-0.08
2,3,4,5,6-Pentafluorotoluene	3.19	2.83	0.36
2,3,4,5-Tetrachloroanisole	5.9	6.24	-0.34
2,3',4,5-Tetrachlorobiphenyl	9.11	8.54	0.57
2,3,4',5-Tetrachlorobiphenyl	8.79	8.54	0.25
2,3',4',5-Tetrachlorobiphenyl	8.87	8.54	0.33
2,3,4,6,7,8-Hexachlorodibenzofuran	10.87	10.74	0.13
2,3',4,6-Tetrabromodiphenyl ether	10.23	9.9	0.33
2,3,4,6-Tetrachloroanisole	6.02	6.24	-0.22
2,3',4,6-Tetrachlorobiphenyl	8.38	8.54	-0.16
2,3,4',6-Tetrachlorobiphenyl	8.38	8.54	-0.16
2,3',4',6-Tetrachlorobiphenyl	8.61	8.54	0.07
2,3,4,6-Tetrachlorophenol	8.01	8.07	-0.06
2,3,4,7,8-Pentachlorodibenzofuran	10.37	10.14	0.23
2,3,4-Tribromoanisole	6.36	6.63	-0.27
2,3,4-Tribromodiphenylether	9.49	8.97	0.52
2,3,4-Trichloroanisole	5.61	5.64	-0.03
2,3',4-Trichlorobiphenyl	8.02	7.94	0.08
2,3,4'-Trichlorobiphenyl	8.33	7.94	0.39
2,3',4'-Trichlorobiphenyl	8.2	7.94	0.26
2',3,4-Trichlorodiphenylether	8.59	7.98	0.61
2,3',4-Trichlorodiphenylether	8.43	7.98	0.45
2,3,4'-Trichlorodiphenylether	8.72	7.98	0.74
2,3,4-Trimethylpentane	3.2	2.63	0.57
2,3,5,6-Tetrabromo-p-xylene	8.85	7.86	0.99
2,3,5,6-Tetrachloroanisole	5.71	6.24	-0.53
2,3,5,6-Tetrachlorobiphenyl	8.18	8.54	-0.36
2,3,5,6-Tetrachloropyridine	5.41	5.93	-0.52
2,3',5-Tribromobiphenyl	9.13	8.93	0.20
2,3,5-Trichloroanisole	5.39	5.64	-0.25
2,3',5'-Trichlorobiphenyl	8.03	7.94	0.09
2,3',5-Trichlorobiphenyl	7.99	7.94	0.05
2,3,5-Trichlorodiphenylether	8.55	7.98	0.57

2,3,5-Trichlorophenol	7.33	7.47	-0.14
2,3,6,7-Tetrachloronaphthalene	8.4	8.12	0.28
2,3,6-Tribromoanisole	6.48	6.63	-0.15
2,3,6-Trichloroanisole	5.22	5.64	-0.42
2,3,6-Trichlorobiphenyl	7.94	7.94	0.00
2,3,6-Trichlorodiphenylether	7.4	7.98	-0.58
2,3,6-Trimethylnaphthalene	6.68	6.56	0.12
2,3,7,8-Tetrachlorodibenzofuran	9.89	9.54	0.35
2,3,7,8-Tetrachlorodibenzo-p-dioxin	10.05	9.58	0.47
2,3,7-Trichlorodibenzo-p-dioxin	9.14	8.98	0.16
2,3,8-Trichlorodibenzofuran	8.93	8.94	-0.01
2,3-Butanedione	2.92	3.48	-0.56
2,3-Butyl dinitrate	4.78	5.06	-0.28
2,3-Butyleneglycol	5.3	5.78	-0.48
2,3-Dibromo-5,6-dichloroanisole	6.64	6.9	-0.26
2,3-Dichloro-1.4-naphthoquinone	7.72	7.68	0.04
2,3-Dichloroanisole	5.06	5.04	0.02
2,3'-Dichlorobiphenyl	7.31	7.34	-0.03
2,3-Dichlorobiphenyl	7.35	7.34	0.01
2,3-Dichlorodibenzofuran	8.3	8.34	-0.04
2,3-Dichlorodibenzo-p-dioxin	8.5	8.38	0.12
2,3-Dichloronitrobenzene	6.55	5.94	0.61
2,3-Dichlorophenol	6.15	6.87	-0.72
2,3-Dichloropropene	3.12	2.6	0.52
2,3-Diethyl-5-methylpyrazine	5.15	5.76	-0.61
2,3-Dimethyl-2-butanol	4.35	4.27	0.08
2,3-Dimethylbutane	1.84	2.16	-0.32
2,3-Naphthalenediol	10.64	10.42	0.22
2,3-Xylenol	6.87	6.49	0.38
2,3-Xylidine	5.77	6.2	-0.43
2,4,4',5-Tetrachlorobiphenyl	8.86	8.54	0.32
2,4,4',5-Tetrachlorodiphenyl ether	7.95	8.58	-0.63
2,4,4',6-Tetrabromodiphenyl ether	10.13	9.9	0.23
2,4,4',6-Tetrachlorobiphenyl	8.09	8.54	-0.45
2,4,4'-Tribromodiphenyl ether	9.46	8.97	0.49
2,4,4'-Trichlorobiphenyl	7.92	7.94	-0.02
2,4,4'-Trichlorodiphenyl ether	7.61	7.98	-0.37
2,4,5-T	9.59	9.13	0.46
2,4',5-Tribromobiphenyl	9.21	8.93	0.28
2,4,5-Trichloroanisole	5.43	5.64	-0.21
2,4,5-Trichlorobiphenyl	7.96	7.94	0.02
2,4',5-Trichlorobiphenyl	7.92	7.94	-0.02

2,4,5-Trichlorodiphenyl ether	7.12	7.98	-0.86
2,4',5-Trichlorodiphenyl ether	8.46	7.98	0.48
2,4,5-Trichlorophenol	6.9	7.47	-0.57
2,4,5-Trimethylaniline	6.15	6.61	-0.46
2,4,5-Trimethylnaphthalene	6.81	6.56	0.25
2,4,6-Collidine	5.15	4.56	0.59
2,4,6-Tribromo-3-chloroanisole	6.64	7.23	-0.59
2,4,6-Tribromoanisole	6.21	6.63	-0.42
2,4,6-Tribromodiphenyl ether	9.02	8.97	0.05
2,4',6-Tribromodiphenyl ether	9.28	8.97	0.31
2,4,6-Trichloroanisole	5.17	5.64	-0.47
2,4,6-Trichlorobiphenyl	7.56	7.94	-0.38
2,4',6-Trichlorobiphenyl	7.74	7.94	-0.20
2,4,6-Trichlorodibenzofuran	8.82	8.94	-0.12
2,4',6-Trichlorodiphenylether	7.49	7.98	-0.49
2,4,6-Trichlorophenol	6.96	7.47	-0.51
2,4,8-Trichlorodibenzofuran	8.82	8.94	-0.12
2,4-Dibromo-3,5-dichloroanisole	6.64	6.9	-0.26
2,4-Dibromo-3-chloroanisole	6.06	6.3	-0.24
2,4-Dibromo-5,6-dichloroanisole	6.35	6.9	-0.55
2,4-Dibromo-5-chloroanisole	6.18	6.3	-0.12
2,4-Dibromoanisole	6.05	5.7	0.35
2,4'-Dibromodiphenyl ether	8.47	8.04	0.43
2,4-Dibromodiphenyl ether	8.37	8.04	0.33
2,4-Dichloroanisole	4.96	5.04	-0.08
2,4'-Dichlorobiphenyl	7.37	7.34	0.03
2,4-Dichlorobiphenyl	7.15	7.34	-0.19
2,4-Dichlorodiphenyl ether	7.7	7.38	0.32
2,4-Dichloronitrobenzene	6.15	5.94	0.21
2,4-Dichlorophenol	6.72	6.87	-0.15
2,4-Dichlorotoluene	5.17	4.93	0.24
2,4-Dimethyl-3-pentanone	3.82	3.54	0.28
2,4-Dimethylpentane	2.63	2.54	0.09
2,4-Dinitrotoluene	6.96	6.57	0.39
2,4-Lutidine	5.22	4.48	0.74
2,4-Xylenol	6.58	6.49	0.09
2,4-Xylidine	5.37	6.2	-0.83
2,5-Dichloroanisole	5	5.04	-0.04
2,5-Dichlorobiphenyl	7.16	7.34	-0.18
2,5-Dimethyl-2,4-hexadiene	3.31	3.22	0.09
2,5-Dimethylhexane	3.1	2.92	0.18
2,5-Dimethylpyrazine	4.69	4.82	-0.13

2,5-Dinitrophenol	7.06	7	0.06
2,5-Dinitrotoluene	6.53	6.57	-0.04
2,5-Hexanediol	7.25	6.64	0.61
2,5-Hexyl dinitrate	5.93	5.92	0.01
2,5-Xylenol	6.54	6.49	0.05
2,5-Xylidine	5.5	6.2	-0.70
2,6-Dibromo-3,4,5-trichloroanisole	6.88	7.5	-0.62
2,6-Dibromo-4-chloroanisole	5.77	6.3	-0.53
2,6-Dibromoanisole	5.37	5.7	-0.33
2,6-Dibromodiphenyl ether	8.12	8.04	0.08
2,6-Dichloro-4-nitroaniline	8.1	8	0.10
2,6-Dichloroanisole	4.55	5.04	-0.49
2,6-Dichlorobenzonitrile	5.71	5.73	-0.02
2,6-Dichlorobiphenyl	7.18	7.34	-0.16
2,6-Dichlorodiphenyl ether	6.82	7.38	-0.56
2,6-Dichlorophenol	6.03	6.87	-0.84
2,6-Dichlorotoluene	5.13	4.93	0.20
2,6-Diisopropylnaphthalene	8.1	7.2	0.90
2,6-Dimethoxyphenol	6.05	6.71	-0.66
2,6-Dimethylnaphthalene	6.3	6.18	0.12
2,6-Dimethyl-N-nitrosomorpholine	5.05	5.31	-0.26
2,6-Dimethylpyrazine	3.8	4.82	-1.02
2,6-Dinitro-4-methylphenol	7.87	7.41	0.46
2,6-Dinitrotoluene	6.99	6.57	0.42
2,6-Lutidine	4.94	4.15	0.79
2,6-Xylenol	6.11	6.49	-0.38
2,6-Xylidine	5.54	6.2	-0.66
2,7-Dichlorodibenzofuran	8.27	8.34	-0.07
2,7-Dichlorodibenzo-p-dioxin	8.36	8.38	-0.02
2,7-Dichloronaphthalene	6.7	6.92	-0.22
2,7-Dimethylnaphthalene	6.14	6.18	-0.04
2,8-Dichlorodibenzofuran	8.36	8.34	0.02
2,8-Dichlorodibenzo-p-dioxin	8.36	8.38	-0.02
2,5-Dichloronitrobenzene	6.27	5.94	0.33
2-Aminoanthraquinone	11.49	11.32	0.17
2-Anisaldehyde	5.94	5.32	0.62
2-Bromo-3,4,5-trichloroanisole	6.35	6.57	-0.22
2-Bromo-3,5-dichloroanisole	5.82	5.97	-0.15
2-Bromo-4,6-dichloroanisole	5.48	5.97	-0.49
2-Bromo-4-chloroanisole	5.26	5.37	-0.11
2-Bromo-6-chloroanisole	4.96	5.37	-0.41
2-Bromoanisole	4.7	4.77	-0.07

2-Bromodiphenyl ether	7.24	7.11	0.13
2-Bromofluorene	8.06	8.46	-0.40
2-Bromopropane	2.48	2.63	-0.15
2-Bromotoluene	4.56	4.66	-0.10
2-Butanol	3.85	3.95	-0.10
2-Butanone	2.79	2.83	-0.04
2-Butylamine	3.61	3.65	-0.04
2-Chloro-2-methylbutane	2.45	2.55	-0.10
2-Chloro-2-methylpropane	1.84	2.12	-0.28
2-Chloro-4-nitroaniline	7.82	7.4	0.42
2-Chloro-6-(trichloromethyl)pyridine	6.21	6.13	0.08
2-Chloroaniline	5.39	5.98	-0.59
2-Chloroanisole	5.1	4.44	0.66
2-Chloroanthracene	8.47	8.72	-0.25
2-Chlorobiphenyl	6.43	6.74	-0.31
2-Chlorobutane	2.38	2.96	-0.58
2-Chlorodibenzofuran	7.67	7.74	-0.07
2-Chlorodibenzo-p-dioxin	7.56	7.78	-0.22
2-Chlorodiphenyl ether	6.42	6.78	-0.36
2-Chloroethanol	4.3	4.12	0.18
2-Chloronaphthalene	5.76	6.32	-0.56
2-Chloronitrobenzene	5.2	5.34	-0.14
2-Chlorophenol	5.4	6.27	-0.87
2-Chloropropane	2.05	2.53	-0.48
2-Chloropyridine	4.37	4.36	0.01
2-Chlorotoluene	4.11	4.33	-0.22
2-Cresyl diphenyl phosphate	10.7	10.39	0.31
2-Decanone	5.48	5.41	0.07
2-Ethoxyethanol	4.12	4.39	-0.27
2-Ethoxyethylacetate	4.43	4.03	0.40
2-Ethyl-1-hexanol	5.58	5.63	-0.05
2-Ethyl-3-methoxypyrazine	4.92	5.4	-0.48
2-Ethylaniline	5.43	6.22	-0.79
2-Ethylbutanoic acid	5.72	5.94	-0.22
2-Ethylhexanoic acid	6.28	6.8	-0.52
2-Ethylhexyl 2-(2,4-dichlorophenoxy)acetate	9.12	9.29	-0.17
2-Ethylhexyl 2-(4-chloro-2-methylphenoxy)acetate	9.83	9.1	0.73
2-Ethylhexyl 2,3,4,5-tetrabromobenzoate	10.43	11.4	-0.97
2-Ethylhexyl acetate	6.11	5.27	0.84
2-Ethylhexylamine	5.19	5.41	-0.22
2-Ethyl-naphthalene	6.12	6.2	-0.08
2-Ethylpyridine	4.76	4.5	0.26

2-Ethyltoluene	4.23	4.3	-0.07
2-Fluoroaniline	4.66	5.2	-0.54
2-Fluoroethanol	1.98	2.64	-0.66
2-Fluorophenol	5.46	5.49	-0.03
2-Heptanol	5.1	5.24	-0.14
2-Heptanone	4.15	4.12	0.03
2-Heptenal	4.55	4.36	0.19
2-Hexanol	4.73	4.81	-0.08
2'-Hydroxy-2,4-dibromodiphenylether	9.23	10.39	-1.16
2-Hydroxy-4-methoxybenzophenone	9.06	8.58	0.48
2-Hydroxyacetophenone	5.21	5.65	-0.44
2-Hydroxyethylmethacrylate	5.3	5.61	-0.31
2-Iodophenol	7.07	7.5	-0.43
2-Isopropoxyethanol	4.65	4.57	0.08
2-Isopropyl-5-methylphenol	7.05	7.06	-0.01
2-Isopropylaniline	5.59	6.36	-0.77
2-Isopropyl-naphthalene	6.21	6.31	-0.10
2-Isopropyltoluene	4.84	4.41	0.43
2'-Methoxy-2,3',4,5'-tetrabromodiphenylether	10.57	10.42	0.15
2'-Methoxy-2,4,4'-tribromodiphenylether	10.1	9.49	0.61
2-Methoxyacetophenone	6.27	5.33	0.94
2-Methoxyaniline	5.26	5.9	-0.64
2-Methoxyethylamine	3.81	3.87	-0.06
2-Methoxynitrobenzene	5.4	5.26	0.14
2-Methoxyphenol	5.26	6.19	-0.93
2-Methyl-1-butanol	4.41	4.34	0.07
2-Methyl-1-propanol	3.93	3.91	0.02
2-Methyl-2-butanol	4.01	4.13	-0.12
2-Methyl-2-propanol	3.5	3.7	-0.20
2-Methyl-3-buten-2-ol	3.89	3.99	-0.10
2-Methylacrylonitrile	2.6	2.73	-0.13
2-Methylbenzaldehyde	4.88	5.21	-0.33
2-Methylbutyric acid	5.24	5.51	-0.27
2-Methylfuran	2.43	2.85	-0.42
2-Methylnaphthalene	5.11	5.8	-0.69
2-Methylpentane	2.34	2.45	-0.11
2-Methylpropane	1.23	1.69	-0.46
2-Methylpropanoic acid	5.21	5.08	0.13
2-Methylpropenoic acid	5.65	5.12	0.53
2-Methylpyrazine	4.05	4.74	-0.69
2-Methylquinoline	6.99	6.37	0.62
2-Methylthiophene	3.48	3.4	0.08

2-Naphthol	8.47	8.07	0.40
2-Naphthylamine	7.59	7.78	-0.19
2-n-Hexoxyethanol	5.76	6.11	-0.35
2-Nitroaniline	6.46	5.29	1.17
2-Nitrophenol	5.05	5.58	-0.53
2-Nitrotoluene	4.87	5.15	-0.28
2-Nonanone	5.03	4.98	0.05
2-Nonenal	4.41	5.22	-0.81
2-Octanol	5.67	5.67	0.00
2-Octanone	4.44	4.55	-0.11
2-Pentanol	4.29	4.38	-0.09
2-Phenoxyethanol	5.86	6.16	-0.30
2-Picoline	4.3	4.07	0.23
2-Propanol	3.41	3.52	-0.11
2-Propynyl-(2E,4E)-3,7,11-trimethyl-2,4-dodecadienoate	8.19	7.88	0.31
2-s-Butylphenol	6.68	7.08	-0.40
2-Tolunitrile	4.69	4.94	-0.25
2-Undecanone	5.73	5.84	-0.11
3,3,4,4,5,5,6,6,6-Nonafluorohexan-1-ol	4.54	4.47	0.07
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol	5.26	4.93	0.33
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctyl prop-2-enoate	4.67	4.79	-0.12
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Heptadecafluorodecan-1-ol	5.56	5.39	0.17
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Heptadecafluorodecyl prop-2-enoate	5.34	5.25	0.09
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-Henicosafuorododecan-1-ol	5.71	5.85	-0.14
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,12-Henicosafuorododecyl prop-2-enoate	5.68	5.71	-0.03
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12,13,13,14,14,14-Pentacosafuorotetradecan-1-ol	6.16	6.31	-0.15
3,3',4,4',5,5'-Hexachlorobiphenyl	11.02	9.74	1.28
3,3',4,4',5-Pentabromodiphenyl ether	12	10.83	1.17
3,3',4,4',5-Pentachlorobiphenyl	10.31	9.14	1.17
3,3',4,4',5-Pentachlorodiphenyl ether	8.74	9.18	-0.44
3,3',4,4'-Tetrabromodiphenyl ether	10.7	9.9	0.80
3,3',4,4'-Tetrachlorobiphenyl	9.29	8.54	0.75
3,3',4,4'-Tetrachlorodiphenyl ether	8.7	8.58	0.12
3,3',4-Tribromodiphenyl ether	9.61	8.97	0.64
3,3',4-Trichlorodiphenylether	8.69	7.98	0.71
3,3',5,5'-Tetrachlorobiphenyl	7.7	8.54	-0.84
3,3',5-Trichlorobiphenyl	8.21	7.94	0.27
3,3,5-Trimethylcyclohexyl salicylate	8.56	8.34	0.22

3,3'-Dichlorobiphenyl	7.66	7.34	0.32
3,4,4',5-Tetrachlorobiphenyl	9.67	8.54	1.13
3,4,4'-Tribromodiphenyl ether	9.68	8.97	0.71
3,4,4'-Trichlorobiphenyl	8.64	7.94	0.70
3,4,4'-Trichlorodiphenylether	8.71	7.98	0.73
3,4,5,6-Tetrachloroguaiacol	8.02	8.59	-0.57
3,4,5-Trichloroanisole	5.58	5.64	-0.06
3,4,5-Trichlorocatechol	9.36	9.82	-0.46
3,4',5-Trichlorodiphenylether	8.51	7.98	0.53
3,4,5-Trichloroguaiacol	8.02	7.99	0.03
3,4,5-Trichloroveratrole	6.84	6.16	0.68
3,4'-Dibromodiphenyl ether	8.57	8.04	0.53
3,4-Dibromodiphenyl ether	8.55	8.04	0.51
3,4-Dichloro-1-butene	3.52	3.53	-0.01
3,4-Dichloroaniline	7.05	6.58	0.47
3,4-Dichloroanisole	5.11	5.04	0.07
3,4'-Dichlorobiphenyl	7.47	7.34	0.13
3,4-Dichlorobiphenyl	7.57	7.34	0.23
3,4'-Dichlorodiphenylether	7.75	7.38	0.37
3,4-Dichlorodiphenylether	7.54	7.38	0.16
3,4-Dichlorofluoranthene	10.48	10.7	-0.22
3,4-Dichloronitrobenzene	6.53	5.94	0.59
3,4-Dichlorotoluene	5	4.93	0.07
3,4-Dihydro-4H-pyran	2.07	2.74	-0.67
3,4-Dimethylphenyl N-methylcarbamate	7.29	8.03	-0.74
3,4-Lutidine	5.38	4.81	0.57
3,4-Xylenol	6.85	6.49	0.36
3,4-Xylidine	5.85	6.2	-0.35
3,5,5-Trimethyl-1-hexanol	5.52	5.36	0.16
3,5,5-Trimethyl-2-cyclohexenone	5.15	4.84	0.31
3,5-Dibromo-4-hydroxybenzonitrile	8.99	8.74	0.25
3,5-Dichloroanisole	4.83	5.04	-0.21
3,5-Dichlorobiphenyl	7.52	7.34	0.18
3,5-Dichlorodiphenylether	7.57	7.38	0.19
3,5-Lutidine	5.22	4.81	0.41
3,5-Xylenol	6.81	6.49	0.32
3,6-Dichlorodibenzofuran	8.33	8.34	-0.01
3,6-Dichloropicolinic acid	9.14	8.23	0.91
3,8-Dichlorofluoranthene	10.32	10.7	-0.38
3,9,10-Trichlorophenanthrene	9.98	9.92	0.06
3,9-Dichlorophenanthrene	9.24	9.32	-0.08
3-Acetylpyridine	6.22	5.48	0.74

3-Aminophenylsulfur pentafluoride	7	6.8	0.20
3-Anisaldehyde	5.64	5.32	0.32
3-Bromo-2,4,6-trichloroanisole	6.06	6.57	-0.51
3-Bromo-2,4-dichloroanisole	5.54	5.97	-0.43
3-Bromo-2,5,6-trichloroanisole	6.07	6.57	-0.50
3-Bromo-2,6-dichloroanisole	5.7	5.97	-0.27
3-Bromoanisole	4.43	4.77	-0.34
3-Bromodiphenyl ether	7.36	7.11	0.25
3-Bromonitrobenzene	6.65	5.67	0.98
3-Bromopyridine	4.81	4.92	-0.11
3-Bromotoluene	4.03	4.66	-0.63
3-Buten-2-one	2.95	2.62	0.33
3-Carene	3.8	4.41	-0.61
3-Chloro-1-propanol	4.81	4.55	0.26
3-Chloro-2-methylpropene	2.46	2.71	-0.25
3-Chloro-4-methylaniline	6.42	6.39	0.03
3-Chloroaniline	6.01	5.98	0.03
3-Chloroanisole	4.92	4.44	0.48
3-Chlorobiphenyl	6.78	6.74	0.04
3-Chlorodibenzofuran	7.67	7.74	-0.07
3-Chlorofluoranthene	9.54	10.1	-0.56
3-Chloronitrobenzene	5.64	5.34	0.30
3-Chlorophenol	7.21	6.27	0.94
3-Chloropyridine	4.17	4.59	-0.42
3-Chlorotoluene	4.15	4.33	-0.18
3-Ethylphenol	6.86	6.51	0.35
3-Ethylpyridine	4.92	4.83	0.09
3-Heptanol	5.08	5.24	-0.16
3-Hexanol	4.54	4.81	-0.27
3-Hydroxy-2,2',4,4',5,6'-hexabromodiphenylether	12.78	14.11	-1.33
3-Hydroxy-2,2',4,4'-tetrabromodiphenylether	11.12	12.25	-1.13
3'-Hydroxy-2,4,4'-tribromodiphenylether	10.29	11.32	-1.03
3'-Hydroxy-2,4-dibromodiphenylether	9.96	10.39	-0.43
3-Hydroxybenzaldehyde	8.02	7.15	0.87
3-Isopropylbiphenyl	6.69	6.67	0.02
3-Isopropyltoluene	5.17	4.41	0.76
3-Methoxy-2,2',4,4',5,6'-hexabromodiphenylether	12.1	12.28	-0.18
3-Methoxy-2,2',4,4'-tetrabromodiphenylether	10.77	10.42	0.35
3-Methoxy-4-hydroxybenzaldehyde	7.37	7.67	-0.30
3-Methoxyacetophenone	6.33	5.33	1.00
3-Methoxyphenol	6.76	6.19	0.57
3-Methyl-2-butanol	4.3	4.09	0.21

3-Methyl-2-butanone	3.04	2.97	0.07
3-Methyl-2-nitrophenol	5.98	5.99	-0.01
3-Methyl-4-nitrophenol	8.29	7.5	0.79
3-Methylbutanoic acid	5.46	5.51	-0.05
3-Methylbutyl nitrate	3.9	4.01	-0.11
3-Methylpentane	1.93	2.45	-0.52
3-Methylpyridine	4.57	4.4	0.17
3-Methylstyrene	4.3	4.09	0.21
3-Methylthiophene	3.01	3.19	-0.18
3-Nitroaniline	7.62	6.8	0.82
3-Nitrotoluene	5.19	5.15	0.04
3-Pentanol	4.28	4.38	-0.10
3-Propyltoluene	5.09	4.7	0.39
3-Pyridinecarbonitrile	5.08	5.2	-0.12
3-Pyridinecarboxaldehyde	5.26	5.47	-0.21
3-t-Butylphenol	7.32	6.67	0.65
3-Trifluoromethylaniline	5.19	5.8	-0.61
4-(2,4-Dichlorophenoxy)butyric acid	10.18	9.39	0.79
4,4'-Bipyridine	7.78	7.48	0.30
4,4'-Dibromobiphenyl	8.5	8	0.50
4,4'-Dibromodiphenyl ether	8.64	8.04	0.60
4,4'-Dichlorobiphenyl	7.63	7.34	0.29
4,5,6-Trichloroguaiacol	6.66	7.99	-1.33
4,5-Dichloroguaiacol	6.94	7.39	-0.45
4,6,6,7,8,8-Hexamethyl-1,3,4,7-tetrahydrocyclopenta[g]isochromene	8.15	8.06	0.09
4,6-Dinitro-o-cresol	6.89	7.41	-0.52
4,7-Dibromobenz[a]anthracene	12.78	12.38	0.40
4-Acetylanisole	6.26	5.33	0.93
4-Acetylpyridine	5.82	5.48	0.34
4-Allyl-2-methoxyphenol	6.48	7.25	-0.77
4-Amino-3,5,6-trichloro-2-pyridinecarboxlic acid	11.5	10.89	0.61
4-Aminophenylsulfur pentafluoride	7.01	6.8	0.21
4-Bromo-2,3,5,6-tetrachloroanisole	6.61	7.17	-0.56
4-Bromo-2,3,6-trichloroanisole	6.07	6.57	-0.50
4-bromo-2,3-Dichloroanisole	5.9	5.97	-0.07
4-Bromo-2,6-dichloroanisole	5.49	5.97	-0.48
4-Bromo-2-chloroanisole	5.26	5.37	-0.11
4-Bromo-3,5-dichloroanisole	5.82	5.97	-0.15
4-Bromoanisole	4.48	4.77	-0.29
4-Bromobiphenyl	7.22	7.07	0.15
4-Bromiodobenzene	5.87	6.08	-0.21

4-Bromophenol	7.67	6.6	1.07
4-Bromotoluene	4.39	4.66	-0.27
4-Carboxyphenol	10.03	9.27	0.76
4-Chloro-2-methylphenol	7.02	6.68	0.34
4-Chloro-2-nitrophenol	5.67	6.18	-0.51
4-Chloro-6-nitro-m-cresol	5.58	6.59	-1.01
4-Chloroaniline	6.02	5.98	0.04
4-Chloroanisole	4.97	4.44	0.53
4-Chlorobiphenyl	6.77	6.74	0.03
4-Chlorodiphenyl ether	6.84	6.78	0.06
4-Chloriodobenzene	5.34	5.75	-0.41
4-Chloro-m-cresol	7.95	6.68	1.27
4-Chloronitrobenzene	5.24	5.34	-0.10
4-Chlorophenol	7.39	6.27	1.12
4-Chlorotoluene	4.15	4.33	-0.18
4-Cyanopyridine	4.68	5.2	-0.52
4-Ethylaniline	5.64	6.22	-0.58
4-Ethylphenol	6.84	6.51	0.33
4-Ethylpyridine	5	4.83	0.17
4-Ethyltoluene	4.28	4.3	-0.02
4-Fluoroaniline	4.77	5.2	-0.43
4-Fluoriodobenzene	4.63	4.97	-0.34
4-Fluorophenol	6.16	5.49	0.67
4-Heptanol	5.08	5.24	-0.16
4-Heptanone	4.13	4.12	0.01
4-Hydroxy-2,2',3,4',5-pentabromodiphenylether	12.01	13.18	-1.17
4-Hydroxy-2,2',3,4'-tetrabromodiphenylether	10.95	12.25	-1.30
4'-Hydroxy-2,2',4,5'-tetrabromodiphenylether	11	12.25	-1.25
4-Hydroxyazobenzene	10.51	10.83	-0.32
4-Iodophenol	8.09	7.5	0.59
4-Isopropylbiphenyl	6.77	6.67	0.10
4-Methoxy-2,2',3,4',5-pentabromodiphenylether	11.62	11.35	0.27
4-Methoxy-2-nitrophenol	5.85	6.1	-0.25
4-Methoxy-4-methyl-2-pentanone	4.4	3.94	0.46
4-Methoxyaniline	6.22	5.9	0.32
4-Methoxybenzaldehyde	6.22	5.32	0.90
4-Methyl-1-pentanol	4.52	4.77	-0.25
4-Methyl-1-pentene	2.1	2.36	-0.26
4-Methyl-2-nitrophenol	5.34	5.99	-0.65
4-Methylacetophenone	5.45	5.22	0.23
4-Methylbenzaldehyde	5	5.21	-0.21
4-Methylcyclohexanone	4.52	4.39	0.13

4-Methylpyridine	4.7	4.4	0.30
4-Nitroanisole	6	5.26	0.74
4-Nitrooxy-1-butanol	6.91	5.89	1.02
4-Nitrooxy-2-butanol	6.23	5.64	0.59
4-Nitrophenylsulfur pentafluoride	5.77	6.16	-0.39
4-Nitrotoluene	4.88	5.15	-0.27
4-Nonylphenol	9.73	9.52	0.21
4-Octanol	5.37	5.67	-0.30
4-Phenylcyclohexene	5.66	5.72	-0.06
4-Propylphenol	7.22	6.94	0.28
4-Pyridinecarboxaldehyde	5.34	5.47	-0.13
4-s-Butyl-2-nitrophenol	6.15	6.99	-0.84
4-t-Butylphenol	7.53	6.67	0.86
4-t-Butyltoluene	4.39	4.4	-0.01
4-t-Octylphenol	8.6	7.69	0.91
4-Vinylcyclohexene	3.79	3.65	0.14
4-Vinylpyridine	4.67	4.62	0.05
5,7-Dibromobenz[a]anthracene	12.83	12.38	0.45
5-Amino-1H-1,2,4-triazole	8.09	7.83	0.26
5-Bromo-2,4-dichloroanisole	5.9	5.97	-0.07
5-Ethylidene-2-norbornene	4.23	4.75	-0.52
5-Fluoro-2-nitrophenol	4.77	5.4	-0.63
5-Isopropyl-2-methylphenol	7.2	7.06	0.14
5-Methyl-2-furaldehyde	4.56	4.59	-0.03
5-Methyl-2-nitrophenol	5.35	5.99	-0.64
5-Nitrooxy-2-pentanol	6.53	6.07	0.46
5-Nonanone	4.8	4.98	-0.18
6,12-Dichlorochrysene	12.08	11.72	0.36
6-Bromo-2,3,4-trichloroanisole	6.05	6.57	-0.52
6-Bromo-2,3-dichloroanisole	5.9	5.97	-0.07
6-Bromobenzo[a]pyrene	12.95	13.23	-0.28
6-Chlorobenzo[a]pyrene	12.76	12.9	-0.14
6-Chlorochrysene	11.3	11.12	0.18
6-Hydroxy-2,2',3,3',4'-pentabromodiphenylether	12.42	13.18	-0.76
6-Hydroxy-2,2',3,4,4'-pentabromodiphenylether	11.95	13.18	-1.23
6-Hydroxy-2,2',3,4,5'-pentabromodiphenylether	12.03	13.18	-1.15
6'-Hydroxy-2,2',4,4',5'-pentabromodiphenylether	12.23	13.18	-0.95
6-Hydroxy-2,3,3',4,4',5'-hexabromodiphenylether	13.29	14.11	-0.82
6-Methoxy-2,2',3,3',4'-pentabromodiphenylether	11.98	11.35	0.63
6-Methoxy-2,2',3,4,5'-pentabromodiphenylether	11.52	11.35	0.17
6'-Methoxy-2,2',4,4',5'-pentabromodiphenylether	11.36	11.35	0.01
6-Methoxy-2,2',4,4'-tetrabromodiphenylether	10.77	10.42	0.35

6-Methoxy-2,3,3',4,4',5-hexabromodiphenylether	12.89	12.28	0.61
7,11-Dibromobenz[a]anthracene	12.62	12.38	0.24
7,12-Dibromobenz[a]anthracene	12.66	12.38	0.28
7,12-Dichlorobenz[a]anthracene	12.05	11.72	0.33
7-Bromobenz[a]anthracene	11.73	11.45	0.28
7-Chlorobenz[a]anthracene	11.34	11.12	0.22
8-Chlorofluoranthene	9.58	10.1	-0.52
9,10-Anthraquinone	8.28	9.26	-0.98
9,10-Dibromoanthracene	10.05	9.98	0.07
9,10-Dichlorophenanthrene	9.3	9.32	-0.02
9,10-Dihydrophenanthrene	7.03	7.43	-0.40
9-Bromoanthracene	8.94	9.05	-0.11
9-Bromophenanthrene	8.87	9.05	-0.18
9-Chloroanthracene	8.47	8.72	-0.25
9-Chlorophenanthrene	8.41	8.72	-0.31
9H-Fluoren-9-one	7.93	8.18	-0.25
Abate	11.56	12.26	-0.70
Acenaphthene	6.52	7.07	-0.55
Acenaphthylene	6.34	7	-0.66
Acetaldehyde	2.23	2.39	-0.16
Acetamide	5.38	5.05	0.33
Acetic acid	4.31	4.51	-0.20
Acetochlor	8.62	8.16	0.46
Acetonitrile	2.31	2.12	0.19
Acetophenone	4.45	4.81	-0.36
Acetylacetone (enol form)	4.06	3.84	0.22
Aclonifen	9.96	8.75	1.21
Acrylic acid	5.01	4.73	0.28
Acticin	12.19	11.34	0.85
Adiponitrile	5.64	4.64	1.00
Alachlor	9.31	8.29	1.02
Aldicarb	8.32	8.05	0.27
Aldrin	8.07	8.36	-0.29
all-trans-1,5,9-Cyclododecatriene	5.43	5.39	0.04
Allyl acetate	3.03	3.2	-0.17
Allyl alcohol	3.66	3.56	0.10
Allyl bromide	2.42	2.66	-0.24
Allyl chloride	1.67	2.32	-0.65
Allyl cyanide	2.95	2.77	0.18
Allyl glycidyl ether	3.99	3.63	0.36
Allyl methacrylate	4.12	3.81	0.31
Allylamine	3.28	3.34	-0.06

alpha-Hexachlorocyclohexane	7.62	8.06	-0.44
alpha-Methylstyrene	4.44	4.07	0.37
alpha-Phellandrene	4.41	4.37	0.04
alpha-Pinene	3.75	4.41	-0.66
alpha-Terpinene	3.9	4.62	-0.72
alpha-Terpineol	6.73	6.44	0.29
Altosid	9.2	8.31	0.89
Ambrette musk	8.11	8.09	0.02
Ametryn	9.52	9.77	-0.25
Amicarbazone	11.04	11.12	-0.08
Aminocarb	8.52	9.11	-0.59
Amyl acetate	4.12	4.27	-0.15
Amyl propionate	4.21	4.7	-0.49
Amylamine	4.39	4.41	-0.02
Amylbenzene	5.26	5.12	0.14
Ancymidol	11.35	11.04	0.31
Aniline	4.48	5.38	-0.90
Anisole	4.01	3.84	0.17
Anthracene	7.71	7.7	0.01
Antor	9.74	10.07	-0.33
Arachic alcohol	12.06	11.08	0.98
Aspirin	8.19	7.11	1.08
Atratone	9.87	9.17	0.70
Atrazine	9.08	8.89	0.19
Azaconazole	10.15	9.86	0.29
Azamethiphos	9.58	9.95	-0.37
Azoxystrobin	13.13	13.04	0.09
Bayleton	10.98	10.66	0.32
Beflubutamid	11.49	11.57	-0.08
Benazolin	10.99	10.42	0.57
Benazolin-ethyl	8.42	8.89	-0.47
Benomyl	11.48	11.09	0.39
Benoxacor	7.85	7.93	-0.08
Benz[a]anthracene	10.28	9.98	0.30
Benz[e]acephenanthrylene	11.34	11.3	0.04
Benzalchloride	5.01	4.98	0.03
Benzaldehyde	4.41	4.8	-0.39
Benzamide	8.31	7.46	0.85
Benzene	2.8	3.14	-0.34
Benzo[a]phenanthrene	9.85	9.98	-0.13
Benzo[a]pyrene	11.56	11.7	-0.14
Benzo[b]fluorene	9.42	9.42	0.00

Benzo[b]triphenylene	12.11	12.26	-0.15
Benzo[e]pyrene	10.72	11.7	-0.98
Benzo[f]quinoline	8.43	8.69	-0.26
Benzo[g,h,i]perylene	12.55	13.42	-0.87
Benzo[k]fluoranthene	11.37	11.3	0.07
Benzoic acid	7.23	6.92	0.31
Benzonitrile	4.46	4.53	-0.07
Benzophosphate	9.91	9.95	-0.04
Benzotrifluoride	3.24	3.74	-0.50
Benzoximate	9.27	9.25	0.02
Benzyl acetate	5.2	5.39	-0.19
Benzyl benzoate	7.94	7.8	0.14
Benzyl butyl phthalate	9.66	10.73	-1.07
Benzyl methyl ether	4.29	4.48	-0.19
beta-Citronellol	6.51	6.27	0.24
beta-HCH	8.74	8.06	0.68
beta-Ionone	6.19	6.23	-0.04
beta-Phellandrene	4.42	4.23	0.19
Bifenazate	10.88	10.59	0.29
Bifenoxy	11.7	10.57	1.13
Bioallethrin	9.94	9.81	0.13
Biphenyl	5.88	5.78	0.10
Bis(2-chloroethyl) ether	3.5	3.93	-0.43
Bitertanol	14.23	13.98	0.25
Borneol	5.69	5.96	-0.27
Bromacil	10.02	9.92	0.10
Bromoacetic acid	6.69	5.63	1.06
Bromobenzene	4.08	4.25	-0.17
Bromobutide	9.01	9.85	-0.84
Bromocyclohexane	3.67	4.26	-0.59
Bromoethane	2.11	2.44	-0.33
Bromofenoxim	13.26	13.94	-0.68
Bromophos	7.18	8.08	-0.90
Bromophos-ethyl	9.22	8.68	0.54
Bromoxynil butyrate	8.62	8.95	-0.33
Bromoxynil heptanoate	9.3	10.24	-0.94
Bromoxynil octanoate	10.26	10.67	-0.41
Bromuconazole	11.07	10.37	0.70
Butachlor	10.12	9.1	1.02
Butamifos	9.52	9.59	-0.07
Butanal	3.39	3.25	0.14
Butanamide	6.39	5.91	0.48

Butane	1.53	1.98	-0.45
Butanedioic acid	9.54	9.76	-0.22
Butanoic acid	5.3	5.37	-0.07
Butenachlor	8.79	9.27	-0.48
Butocarboxim	8.23	7.98	0.25
Butralin	8.18	8.68	-0.50
Buturon	10.27	9.95	0.32
Butyl 4-hydroxybenzoate	9.63	8.6	1.03
Butylate	6.64	6.91	-0.27
Butylbenzene	4.34	4.72	-0.38
Butylcellosolve	4.84	5.25	-0.41
Butylmethylketone	3.68	3.69	-0.01
Butylnitrate	3.34	3.87	-0.53
Butyric acid methylester	3.29	3.54	-0.25
Butyronitrile	3.12	2.98	0.14
Cafenstrole	12.22	11.97	0.25
Camphene	4.04	4.27	-0.23
Camphor	5.21	5.06	0.15
Capraldehyde	5.32	5.83	-0.51
Caproic aldehyde	4.41	4.11	0.30
Caprylene	3.35	3.45	-0.10
Caprylic aldehyde	5.36	4.97	0.39
Carbaril	9.55	9.61	-0.06
Carbazole	8.03	8.3	-0.27
Carbendazim	9.83	10.32	-0.49
Carbofuran	9.24	9.15	0.09
Carbophenothion	10.15	9.85	0.30
Carbophos	7.83	8.52	-0.69
Carvone	5.72	5.43	0.29
Cashmeran	6.43	6.74	-0.31
Celestolide	7.58	8	-0.42
CGA307771	12.4	12.45	-0.05
Chloral	3.44	4.08	-0.64
Chloral hydrate	7.65	7.55	0.10
Chlordane	8.92	8.82	0.10
Chlordimeform	7.22	6.58	0.64
Chlorfenidim	9.01	9.14	-0.13
Chlorimuron-ethyl	13.95	14.57	-0.62
Chlormethine	4.29	4.68	-0.39
Chloroacetic acid	6.34	5.29	1.05
Chloroacetic acid ethylester	3.62	3.76	-0.14
Chloroacetonitrile	3.19	2.9	0.29

Chlorobenzene	3.58	3.92	-0.34
Chlorobenzilate	10.44	11.38	-0.94
Chloroethane	1.78	2.1	-0.32
Chloroethylene	0.9	1.71	-0.81
Chlorophthalim	9.26	9.62	-0.36
Chloropropham	7.94	7.89	0.05
Chlorothalonil	8.11	8.14	-0.03
Chloroxifenidim	11.49	12	-0.51
Chlorpyrifos-methyl	7.97	7.9	0.07
Chlorpyriphos	8.41	8.5	-0.09
Chlorsulfuron	12.84	13.08	-0.24
Chlorthion	8.55	7.97	0.58
Chlortoluron	9.92	9.55	0.37
Chlozolate	9.04	9.24	-0.20
Ciafos	6.96	7.16	-0.20
Cimetacarb	11.24	11.09	0.15
Cinmethylin	9.12	8.4	0.72
cis-1,1,1,4,4,4-Hexafluoro-2-butene	1.55	2.02	-0.47
cis-1,2-Cyclohexyl dinitrate	6.4	6.26	0.14
cis-1,2-Dichloroethylene	2.6	2.34	0.26
cis-1,3-Cyclohexyl dinitrate	6.49	6.26	0.23
cis-1,3-Dichloropropene	2.68	2.45	0.23
cis-1,4-Dichloro-2-butene	4.04	3.56	0.48
cis-2,4-Pentyl dinitrate	5.43	5.49	-0.06
cis-2,5-Dimethyltetrahydrofuran	3.28	3.18	0.10
cis-2-Butene	1.43	1.88	-0.45
cis-Nonachlor	9.66	9.6	0.06
Clodinafop-propargyl	10.69	9.93	0.76
Clofenotane	9.88	9.6	0.28
Clofenvinfos	9.78	9.42	0.36
Cloquintocet-mexyl	10.93	11.27	-0.34
Codlure	7.28	7.28	0.00
Colamine	6.32	5.14	1.18
Coronene	14.69	15.14	-0.45
Coumaphos	9.5	10.15	-0.65
Coumarin	6.59	6.25	0.34
Coumatetralyl	13.34	13.4	-0.06
Crotonic acid	5.28	5.19	0.09
Crotoxyphos	9.55	9.29	0.26
Cryofluorane	1.29	1.42	-0.13
Cumene	3.98	4.03	-0.05
Cumyluron	13.22	13.5	-0.28

Cyanazine	9.93	9.64	0.29
Cyanoethylene	2.28	2.34	-0.06
Cycloate	7.36	7.5	-0.14
Cyclododecanol	7.62	7.07	0.55
Cycloheptane	3.49	3.35	0.14
Cyclohexane	2.71	3.08	-0.37
Cyclohexanol	5.18	5.15	0.03
Cyclohexanone	3.99	4.25	-0.26
Cyclohexene	2.83	3.35	-0.52
Cyclohexylamine	5.13	4.85	0.28
Cyclooctane	3.86	3.62	0.24
Cyclopentadecanone	6.59	7.13	-0.54
Cyclopentane	2.21	2.81	-0.60
Cyclopentanol	4.57	4.83	-0.26
Cyclopentanone	3.67	3.93	-0.26
Cyclopropane	1.21	2.27	-1.06
Cyenopyrafen	12.24	12.37	-0.13
Cyfluthrin	11.69	12.14	-0.45
Cymperator	11.37	12.32	-0.95
Cyprazine	10.12	9.66	0.46
Cyproconazole	10.32	11.18	-0.86
Cyprodinil	9.37	9.47	-0.10
Cyromazine	10.97	10.89	0.08
DBCP	4.56	4.53	0.03
DCPA	8.51	9.26	-0.75
DDD	9.87	9.16	0.71
DDE	9.24	9.28	-0.04
Decabromodiphenyl ether	16.12	15.48	0.64
Decamethylcyclopentasiloxane	4.95	5.06	-0.11
Decamethyltetrasiloxane	4.64	4.56	0.08
Decylbenzene	7.43	7.12	0.31
delta-HCH	8.84	8.06	0.78
Demeton-S-methyl	7.32	7.56	-0.24
Desmedipham	12.86	12.94	-0.08
Desmetryn	9.52	10.26	-0.74
Devrinol	10.62	10.72	-0.10
Diallylamine	4	3.64	0.36
Dibenz[a,h]anthracene	12.59	12.26	0.33
Dibenzo[b,d]thiophene	7.28	7.96	-0.68
Dibenzo[b,e]pyridine	8.35	8.59	-0.24
Dibenzofuran	6.59	7.14	-0.55
Dibenzo-p-dioxin	6.57	7.18	-0.61

Dibenzyl ether	6.82	7.19	-0.37
Dibutyl ether	3.89	4.09	-0.20
Dibutyl phthalate	8.66	9.18	-0.52
Dibutylamine	5.17	4.92	0.25
Dicapthon	8.49	7.97	0.52
Dichlofenthion	8.03	7.75	0.28
Dichlorfenidim	10.14	9.74	0.40
Diclofop-methyl	9.5	9.74	-0.24
Dicofol	11.45	11.41	0.04
Diethion	10.01	9.78	0.23
Diethofencarb	10.1	8.93	1.17
Diethyl adipate	6.3	6.36	-0.06
Diethyl cellosolve	3.13	3.42	-0.29
Diethyl malonate	5.01	5.07	-0.06
Diethyl oxalate	4.41	4.64	-0.23
Diethyl phthalate	7.31	7.46	-0.15
Diethyl succinate	5.69	5.5	0.19
Diethyl sulfate	4.6	5.02	-0.42
Diethyl sulphide	3.01	3.34	-0.33
Diethylamine	3.42	3.2	0.22
Diethylcarbonate	3.55	3.74	-0.19
Diethylene glycol monohexyl ether	6.62	7.16	-0.54
Diethyleneglycol dinitrate	5.59	5.75	-0.16
Diethyleneglycol monobutyl ether	6.81	6.3	0.51
Diethyleneglycol-di-n-butylether	5.79	6.19	-0.40
Diethylketone	3.2	3.26	-0.06
Difenoconazole	13.05	12.9	0.15
Difenoxyuron	12.95	11.92	1.03
Diffubenzuron	11.01	11.88	-0.87
Diffumetorim	9.95	9.5	0.45
Dihexyl phthalate	10.43	10.9	-0.47
Diisoamyl ether	4.58	4.37	0.21
Diisobutyl ether	3.4	3.51	-0.11
Diisobutylamine	4.64	4.34	0.30
Diisobutylene	2.79	2.71	0.08
Diisopropyl ether	2.66	2.73	-0.07
Diisopropyl methylphosphonate	5.57	5.55	0.02
Diisopropyl sulfide	3.73	3.2	0.53
Diisopropylamine	3.68	3.4	0.28
Dimepiperate	9.75	9.65	0.10
Dimethachlor	8.94	8.3	0.64
Dimethametryn	10.17	10.34	-0.17

Dimethenamid	8.37	8.27	0.10
Dimethoxymethane	2.39	2.38	0.01
Dimethyl hexanedioate	5.87	5.76	0.11
Dimethyl maleate	4.86	4.72	0.14
Dimethyl malonate	4.68	4.47	0.21
Dimethyl oxalate	3.52	4.04	-0.52
Dimethyl phthalate	6.8	6.86	-0.06
Dimethyl succinate	4.99	4.9	0.09
Dimethyl sulfate	4.81	4.42	0.39
Dimethyl sulfide	2.95	2.98	-0.03
Dimethyl-(2,2-dichlorovinyl) phosphate	5.95	5.24	0.71
Dimethylacetamide	5.33	4.48	0.85
Dimethylamine	2	2.36	-0.36
Dimethylether	1.37	1.77	-0.40
Dimethylterephthalate	6.81	6.86	-0.05
Dimethylvinphos	8.85	8.82	0.03
Dimoxystrobin	12.65	12.25	0.40
Dimpylate	7.97	8.2	-0.23
Dinitramine	8.52	7.95	0.57
Dinoseb	8.05	8.41	-0.36
Di-n-propyl phthalate	7.9	8.32	-0.42
Diofenolan	10.35	9.74	0.61
Dioxacarb	9.52	9.75	-0.23
Diphenyl 2-ethylhexyl phosphate	10.56	10.8	-0.24
Diphenyl ether	6.27	6.18	0.09
Diphenylamine	7.64	7.34	0.30
Diphenylcarbonate	6.93	7.82	-0.89
Diphenylmethane	6.11	6.18	-0.07
Diphenylmethanol	8.46	8.34	0.12
Dipropetryn	9.87	10.05	-0.18
Dipropyl ether	2.97	3.23	-0.26
Dipropylamine	3.59	4.06	-0.47
Disperse Red 1	14.66	14.25	0.41
Disugran	8.83	8.64	0.19
Disulfoton	7.82	7.46	0.36
Dithianon	11.62	11.9	-0.28
Dodecamethylcyclohexasiloxane	5.77	5.78	-0.01
Dodecane	4.88	5.02	-0.14
Dyrene	8.41	8.7	-0.29
Ebufos	8.12	8.24	-0.12
Eicosane	8.42	8.06	0.36
Enanthic acid	6.81	6.66	0.15

Endosulfan sulfate	9.68	9.67	0.01
Endrin	9.02	8.68	0.34
endrin aldehyde	9.47	9.16	0.31
Endrin ketone	10.11	9.69	0.42
Enzacamene	8.53	8.63	-0.10
Epichlorohydrin	3.21	3.14	0.07
EPN	10.31	10.61	-0.30
epsilon-Caprolactam	7.08	6.8	0.28
Eradicane	6.3	6.63	-0.33
Erythritol	10.25	9.94	0.31
Esprocarb	8.29	8.85	-0.56
Ethane	0.42	1.22	-0.80
Ethanol	3.2	3.34	-0.14
Ethene	0.28	1.02	-0.74
Ethiofencarb	9.12	9.64	-0.52
Ethoxybenzene	4.12	4.14	-0.02
Ethychlozate	9.85	10.31	-0.46
Ethyl 4-hydroxybenzoate	8.9	7.74	1.16
Ethyl acetate	2.7	2.98	-0.28
Ethyl acetoacetate	4.36	4.49	-0.13
Ethyl acrylate	3.12	3.2	-0.08
Ethyl benzoate	5.26	5.39	-0.13
Ethyl butanoate	3.56	3.84	-0.28
Ethyl ether	2.19	2.37	-0.18
Ethyl formate	2.19	2.24	-0.05
Ethyl hexanoate	4.42	4.7	-0.28
Ethyl iodide	2.59	2.52	0.07
Ethyl methacrylate	3.34	3.59	-0.25
Ethyl methyl sulfide	2.61	3.16	-0.55
Ethyl propanoate	3.15	3.41	-0.26
Ethyl t-butyl ether	2.69	2.73	-0.04
Ethyl trans-cinnamate	6.67	6.07	0.60
Ethyl vanillin	7.49	7.97	-0.48
Ethyl vinyl ether	1.71	1.61	0.10
Ethylamine	2.96	3.12	-0.16
Ethylbenzene	3.72	3.92	-0.20
Ethylcyclohexane	3.57	3.55	0.02
Ethylene dodecanedioate	7.75	7.76	-0.01
Ethylenediamine	4.49	4.92	-0.43
Ethylenedichloride	2.78	2.88	-0.10
Ethylpyrazine	4.48	5.17	-0.69
Ethyne	0.33	0.5	-0.17

Ethynylbenzene	4.11	3.78	0.33
Etofenprox	12.48	11.46	1.02
Etohexadiol	6.65	7.46	-0.81
Etoxazole	11.53	11.68	-0.15
Etrimfos	8.07	7.91	0.16
Fenamidone	10.87	11.2	-0.33
Fenazaquin	10.29	10.75	-0.46
Fenbuconazole	10.91	11.11	-0.20
Fenchlorphos	7.61	7.75	-0.14
Fenchol	6.06	5.96	0.10
Fenclorim	7.32	7.76	-0.44
Fenhexamid	11.77	12.78	-1.01
Fenobucarb	8.19	8.62	-0.43
Fenothiocarb	9.24	8.61	0.63
Fenoxycarb	11.93	11.27	0.66
Fenpiclonil	10.37	9.61	0.76
Fenpropidin	9.38	8.72	0.66
Fenpropimorph	8.69	8.84	-0.15
Fenpyroximate	9.32	9.17	0.15
Fenthion	8.2	7.77	0.43
Fenthoate	8.54	8.84	-0.30
Fentrazamide	11.48	11.38	0.10
Fenvalerate	12.98	13.38	-0.40
Ferimzone	10.88	10.78	0.10
Flamprop-M-isopropyl	9.71	10.72	-1.01
Flamprop-M-methyl	9.54	10.24	-0.70
Flonicamid	10.26	9.79	0.47
Fluacrypyrim	10.15	10.74	-0.59
Fluazifop-butyl	10.3	10.5	-0.20
Flucythrinate	12.09	12.85	-0.76
Flufenoxuron	14.74	14.98	-0.24
Fluometuron	9.12	8.96	0.16
Fluopyram	10.99	11.01	-0.02
Fluoranthene	8.88	9.02	-0.14
Fluorene	6.9	7.14	-0.24
Fluoroacetone	2.35	1.7	0.65
Fluorobenzene	2.84	3.14	-0.30
Fluquinconazole	11.58	12.05	-0.47
Fluridone	9.81	10.04	-0.23
Flurochloridone	9.01	8.74	0.27
Flurprimidol	10.41	10.7	-0.29
Flusulfamide	10.74	10.48	0.26

Fluthiamide	9.27	9.83	-0.56
Flutolanil	11.28	10.84	0.44
Flutriafol	10.59	10.82	-0.23
Fluxapyroxad	12.22	12.31	-0.09
Fluxofenim	7.4	7.49	-0.09
Folbex	11.73	12.22	-0.49
Forchlorfenuron	12.85	12.11	0.74
Formaldehyde diethylacetal	3.29	2.98	0.31
Formic acid	4.06	3.77	0.29
Formothion	7.85	8.42	-0.57
Furalaxyl	9.66	9.76	-0.10
Furan	1.95	2.18	-0.23
Furfural	3.96	3.92	0.04
Fyrol FR-2	10.6	10.79	-0.19
gamma-Terpinene	4.28	4.73	-0.45
Glycerol trinitrate	6.87	6.57	0.30
Glyceryltriacetate	6.42	6.48	-0.06
Glycidyl butyl ether	3.44	4.27	-0.83
Glyme	3.12	2.82	0.30
Guajen	6.51	6.18	0.33
Haloxyfop-etotyl	12.14	11.29	0.85
Haloxyfop-P-methyl	9.29	9.94	-0.65
Harmony	13.84	13.67	0.17
Hemimellitene	4.61	4.28	0.33
Heptachlor	7.7	8.19	-0.49
Heptachlor epoxide	8.62	8.51	0.11
Heptane	2.93	3.12	-0.19
Heptanedioic acid	10.69	11.05	-0.36
Heptenophos	7.5	7.74	-0.24
Heptyl bromide	4.26	4.59	-0.33
Heptylbenzene	6.3	5.92	0.38
Heroine	11.79	12.74	-0.95
Hexabromobenzene	9.53	8.9	0.63
Hexachlorobenzene	7.55	6.92	0.63
Hexachlorobutadiene	4.58	4.98	-0.40
Hexachloroethane	4.47	4.7	-0.23
Hexaconazole	10.79	11.26	-0.47
Hexaflumuron	13.09	13.44	-0.35
Hexafluoro-2-propanol	4.34	3.54	0.80
Hexafluorobenzene	2.11	2.24	-0.13
Hexamethylbenzene	6.31	5.42	0.89
Hexamethyldisiloxane	2.71	2.68	0.03

Hexane	2.4	2.74	-0.34
Hexanenitrile	4.08	3.84	0.24
Hexazinone	11.07	10.95	0.12
Hexyl bromide	3.77	4.16	-0.39
Hexylbenzene	5.83	5.52	0.31
Hydrocinnamyl alcohol	6.79	6.61	0.18
Hydroxyacetic acid	6.08	6.53	-0.45
Imibenconazole	12.92	12.74	0.18
Imiprothrin	11.24	11.71	-0.47
Indane	4.28	5.08	-0.80
Indanofan	11.06	12.12	-1.06
Indeno[1,2,3-cd]pyrene	12.43	13.02	-0.59
Indole	6.95	6.36	0.59
Indoxacarb	14.14	14.01	0.13
Iodobenzene	4.55	5.15	-0.60
Ioxynil	11.31	10.54	0.77
Ipconazole	11.06	11.96	-0.90
Isazofos	8.11	8.21	-0.10
Isoamyl acetate	3.94	3.98	-0.04
Isobutene	1.46	1.81	-0.35
Isobutyl acetate	3.45	3.55	-0.10
Isobutyl acrylate	3.71	3.77	-0.06
Isobutyl methacrylate	4.31	4.16	0.15
Isobutyl methyl ketone	3.3	3.4	-0.10
Isobutylbenzene	4.01	4.43	-0.42
Isobutyronitrile	2.87	2.69	0.18
Isocumene	4.09	4.32	-0.23
Isofenphos	9.63	9.58	0.05
Isoprene	2.06	2	0.06
Isoprocab	8.02	8.19	-0.17
Isopropazol	9.67	10.25	-0.58
Isopropyl (2,4-dichlorophenoxy)acetate	6.21	7.18	-0.97
Isopropyl propionate	3.16	3.59	-0.43
Isopropylacetate	2.93	3.16	-0.23
Isoproturon	10.18	9.52	0.66
Isopyrazam (syn form)	13.95	13.72	0.23
Isoquinoline	6.16	6.39	-0.23
Isouron	9.51	9.87	-0.36
Isoxathion	8.48	8.31	0.17
Isoxazole	2.9	2.55	0.35
Jodfenphos	9.09	8.98	0.11
Kappa-Tefluthrin	7.79	7.59	0.20

Karbutilate	12.88	12.9	-0.02
Kitazin	8.98	8.91	0.07
Kresoxim-methyl	9.84	9.45	0.39
KTU3616	10.44	11.24	-0.80
lambda-Cyhalothrin	12.11	11.74	0.37
Lenacil	12.21	12.05	0.16
Leptophos	11.31	11.02	0.29
Limonene oxide	5.75	4.78	0.97
Linalool	5.97	5.85	0.12
Lindane	7.48	8.06	-0.58
L-Menthone	5.18	5.1	0.08
Lysodren	9.57	9.16	0.41
Malic acid	9.9	10.02	-0.12
m-Anisidine	6.07	5.9	0.17
m-Anthranilic acid	9.89	8.98	0.91
m-Cresol	6.28	6.08	0.20
Mecoprop	9.74	8.52	1.22
Mefenacet	10.29	10.46	-0.17
Menthol	6.08	6	0.08
Mepanipirim	9.38	9.57	-0.19
Meptyldinocap	12.17	11.67	0.50
Mercaptodimethur	9.71	9.44	0.27
Metalaxyl	9.28	8.98	0.30
Metamitron	10.85	10.53	0.32
Metconazole	10.57	11.41	-0.84
Methacrylamide	6.74	5.66	1.08
Methanol	2.84	3.04	-0.20
Methibenzuron	10.04	10.13	-0.09
Methidathion	8.74	8	0.74
Methoprotetryne	10.63	10.95	-0.32
Methoxychlor	10.57	9.44	1.13
Methoxyflurane	3.03	3.77	-0.74
Methyl (Z) 9-octadecenoate	9.59	9.38	0.21
Methyl 2-hydroxybenzoate	5.86	5.93	-0.07
Methyl 4-hydroxybenzoate	8.57	7.44	1.13
Methyl acetate	2.31	2.68	-0.37
Methyl acrylate	2.8	2.9	-0.10
Methyl benzoate	4.92	5.09	-0.17
Methyl cellosolve	3.76	4.09	-0.33
Methyl decanoate	5.94	6.12	-0.18
Methyl formate	1.75	1.94	-0.19
Methyl hexanoate	4.22	4.4	-0.18

Methyl isoamyl ketone	3.97	3.83	0.14
Methyl laurate	6.84	6.98	-0.14
Methyl methacrylate	3.08	3.29	-0.21
Methyl pivalate	3.55	3.27	0.28
Methyl propanoate	2.9	3.11	-0.21
Methyl t-pentyl ether	2.98	2.86	0.12
Methyl trifluoroacetate	1.58	2.69	-1.11
Methyl valerate	3.8	3.97	-0.17
Methylacetamide	5.4	5.07	0.33
Methylamine	2.55	2.7	-0.15
Methylbenzene	3.31	3.52	-0.21
Methylchloroform	2.7	3.01	-0.31
Methylcyanoacetate	4.17	3.91	0.26
Methylcyclohexane	3.03	3.17	-0.14
Methylcyclopentane	2.35	2.9	-0.55
Methylcyclopropylketone	3.71	3.64	0.07
Methylnitrophos	7.62	7.78	-0.16
Methyl-n-propylketone	3.19	3.26	-0.07
Methyloxiran	2.36	2.36	0.00
Methylparathion	7.34	7.37	-0.03
Methylpropylether	2.49	2.5	-0.01
Metofluthrin	8.54	8.05	0.49
Metolachlor	9.37	8.83	0.54
Metolcarb	6.71	7.62	-0.91
Metominostrobin	9.85	9.55	0.30
Metoxuron	10.35	9.66	0.69
Metribuzin	9.15	8.65	0.50
Metsulfovax	10.08	10.44	-0.36
Metsulfuron-methyl	13.82	14.25	-0.43
Milbemectin A3	17.15	17.24	-0.09
Mocap	8.51	8.38	0.13
Molinate	7.06	6.86	0.20
Monalide	9.71	9.06	0.65
Monocrotophos	9.37	8.79	0.58
Morpholine	4.04	3.73	0.31
Moskene	8.31	8.92	-0.61
MTBE	2.48	2.43	0.05
m-Toluidine	5.42	5.79	-0.37
Musk ketone	8.77	9.47	-0.70
Musk tebetine	8.3	8.39	-0.09
Musk xylene	8.24	9.4	-1.16
Myclobutanil	9.51	9.67	-0.16

Myrcene	4.08	3.78	0.30
Myristyl alcohol	8.49	8.5	-0.01
N,N-Diethylaniline	5.56	5.65	-0.09
N,N-Dimethylaniline	4.78	4.81	-0.03
N,N-Dimethylbenzylamine	5	5.11	-0.11
N,N-Dimethylformamide	4.38	4.18	0.20
N,N-Dimethyl-p-toluidine	5.46	5.22	0.24
n-Amyl ether	4.8	4.95	-0.15
Naphthalene	5.37	5.42	-0.05
n-Butyl acetate	3.65	3.84	-0.19
n-Butyl acrylate	4.05	4.06	-0.01
n-Butyl methyl ether	2.77	2.93	-0.16
n-Butylbenzoate	6.25	6.25	0.00
n-Butylmethacrylate	4.41	4.45	-0.04
n-Decanoic acid	8.31	7.95	0.36
n-Decyl alcohol	6.81	6.78	0.03
Neohexane	2.09	2.04	0.05
Neopentyl alcohol	4.06	3.93	0.13
Neral	5.43	5.39	0.04
N-Ethylaniline	5.46	5.82	-0.36
n-Heptaldehyde	4.74	4.54	0.20
n-Heptylamine	5.29	5.27	0.02
n-Hexanoic acid	6.31	6.23	0.08
n-Hexylacetate	4.58	4.7	-0.12
n-Hexylamine	4.88	4.84	0.04
Niclofen	8.57	8.8	-0.23
Nitrobenzene	4.58	4.74	-0.16
Nitroethane	2.88	2.67	0.21
N-Methyl-2-pyrrolidone	6.13	5.57	0.56
N-Methyl-3,5-dimethylphenyl carbamate	8.06	8.03	0.03
N-Methylaniline	4.99	5.4	-0.41
N-Methylformamide	5.17	4.77	0.40
N-Methylmorpholine	3.77	3.65	0.12
N-Methylpiperidine	4.05	3.89	0.16
N-Methylpyrrole	3.28	2.94	0.34
N-Methylpyrrolidine	3.64	3.57	0.07
N-Nitrosodibutylamine	5.81	6.3	-0.49
N-Nitrosodiethylamine	4.04	4.58	-0.54
N-Nitrosodiisopropylamine	5.36	4.78	0.58
N-Nitrosodimethylamine	3.72	3.74	-0.02
N-Nitrosodipropylamine	5.57	5.44	0.13
N-Nitrosoethylbutylamine	5.46	5.44	0.02

N-Nitrosohexamethyleneimine	6.16	5.67	0.49
N-Nitrosomorpholine	5.56	5.11	0.45
N-Nitroso-N-methylethylamine	3.85	4.16	-0.31
N-Nitroso-N-methyl-N-butylamine	4.3	5.02	-0.72
N-Nitrosopiperidine	5.19	5.35	-0.16
N-Nitrosopyrrolidine	5.64	5.03	0.61
n-Octanoic acid	7.38	7.09	0.29
n-Octylamine	5.73	5.7	0.03
Nonane	3.9	3.88	0.02
Nopinene	3.68	4.27	-0.59
Norflurazon	10.7	10.91	-0.21
n-Propyl acetate	3.17	3.41	-0.24
n-Propyl iodide	2.96	2.95	0.01
n-Propylformate	2.66	2.67	-0.01
O,O-Dimethyl-S-[2-(ethylthio)ethyl]dithiophosphate	7.52	6.86	0.66
o-Anthranilic acid	8.16	7.47	0.69
o-Cresol	6.11	6.08	0.03
Octachlorodibenzofuran	11.9	11.94	-0.04
Octachlorodibenzo-p-dioxin	13.31	11.98	1.33
Octachloronaphthalene	11.48	10.52	0.96
Octadecane	7.87	7.3	0.57
Octafluoronaphthalene	4.7	4.28	0.42
Octamethylcyclotetrasiloxane	4.22	4.34	-0.12
Octamethyltrisiloxane	3.75	3.62	0.13
Octane	3.3	3.5	-0.20
Octylbenzene	6.42	6.32	0.10
Octylcyanide	5.11	5.13	-0.02
Ofurace	8.57	9.55	-0.98
Orbencarb	8.82	8.78	0.04
Orysastrobin	10.92	11.07	-0.15
o-Toluidine	4.66	5.79	-1.13
Oxabetrinil	7.94	7.68	0.26
Oxadiargyl	9.86	9.72	0.14
Oxadiazon	9.42	9.61	-0.19
Oxirane	1.82	2.18	-0.36
Oxyfluorfen	9.21	9.44	-0.23
Paclobutrazol	10.85	10.31	0.54
p-Anthranilic acid	9.46	8.98	0.48
Paraoxon	8.79	8.46	0.33
p-Benzidine	10.29	10.26	0.03
PCNB	8.48	7.74	0.74
p-Cresol	6.3	6.08	0.22

p-Cresyl diphenyl phosphate	10.6	10.39	0.21
p-Cymene	4.54	4.41	0.13
Pebulate	6.83	7.06	-0.23
Pelargonic acid	7.52	7.52	0.00
Penconazole	9.81	9.02	0.79
Pencycuron	13.91	13.8	0.11
Penfenate	9	8.46	0.54
Penoxalin	8.66	8.93	-0.27
Penoxsulam	13.53	13.3	0.23
Pentabromoanisole	9.01	8.49	0.52
Pentabromobenzene	8.3	7.97	0.33
Pentabromotoluene	9.61	8.38	1.23
Pentachloroanisole	6.65	6.84	-0.19
Pentachlorobenzene	6.75	6.32	0.43
Pentachloroethane	4.38	4.26	0.12
Pentachlorophenol	9.01	8.67	0.34
Pentachlorotoluene	7.25	6.73	0.52
Pentafluorobenzene	2.54	2.42	0.12
Pentafluorophenol	4.42	4.77	-0.35
Pentamethylbenzene	6.12	5.04	1.08
Pentane	1.95	2.36	-0.41
Pentanedioic acid	9.88	10.19	-0.31
Pentanenitrile	3.6	3.41	0.19
Pentanoic acid	5.94	5.8	0.14
Perchlordecone	9.12	9.36	-0.24
Perchlorobiphenyl	11.61	12.14	-0.53
Perchlorocyclopentadiene	5.42	5.18	0.24
Perfluorobiphenyl	4.97	4.34	0.63
Perylene	11.7	11.7	0.00
Pethoxamid	8.91	9.48	-0.57
Phantolide	7.76	7.71	0.05
Phenanthrene	7.62	7.7	-0.08
Phenanthridine	9.55	8.69	0.86
Phenethyl alcohol	6.16	6.18	-0.02
Phenmedipham	13.4	13.05	0.35
Phenol	6.06	5.67	0.39
Phenothrin	11.7	10.86	0.84
Phenylacetonitrile	4.99	4.96	0.03
Phenylhydrazine	7.71	7.95	-0.24
Phenylmethanol	5.78	5.75	0.03
Phlorol	6.49	6.51	-0.02
Phosphamide	8.27	8.59	-0.32

Phthalic anhydride	7.54	6.82	0.72
Phthalide	7.75	8.23	-0.48
Phthalthrin	12.14	12.15	-0.01
Picoxystrobin	10.05	9.63	0.42
p-Imazamethabenzmethyl	10.78	10.86	-0.08
Pinacolone	3.24	2.99	0.25
Pinoxaden	12.34	12.44	-0.10
Piperazine	3.77	4.56	-0.79
Piperidine	4.04	3.97	0.07
Piperophos	10.54	11.17	-0.63
Pirimicarb	8.9	9.04	-0.14
Pirimiphos-ethyl	9.39	9.4	-0.01
Pirimiphos-methyl	9.05	8.8	0.25
Plinol	5.88	5.9	-0.02
p-Menthane	4.06	3.73	0.33
Preforan	9.64	9.44	0.20
Prehnitene	4.4	4.66	-0.26
Pretilachlor	9.93	9.89	0.04
Prochloraz	10.16	10.8	-0.64
Procymidone	8.98	8.65	0.33
Profenofos	10.1	9.57	0.53
Promecarb	8.4	8.6	-0.20
Prometon	9.71	9.27	0.44
Prometryn	9.84	9.87	-0.03
Pronamide	9.66	9.44	0.22
Propachlor	7.36	6.83	0.53
Propafos	9.22	9.31	-0.09
Propamocarb	8.07	7.83	0.24
Propanal	3.02	2.82	0.20
Propanamide	5.85	5.48	0.37
Propandioic acid	8.81	7.82	0.99
Propane	0.97	1.6	-0.63
Propanenitrile	2.69	2.55	0.14
Propanoic acid	4.85	4.94	-0.09
Propanone	2.36	2.4	-0.04
Propaquizafop	14.29	13.71	0.58
Propazine	9.02	8.99	0.03
Propenal	2.6	2.61	-0.01
Propham	7.33	7.29	0.04
Propiconazole	10.75	10.9	-0.15
Propisochlor	8.53	8.55	-0.02
Propoxur	8.32	8.21	0.11

Propyl 2-hexyl-3-oxocyclopentanecarboxylate	8.59	8.45	0.14
Propyl 4-hydroxybenzoate	9.48	8.17	1.31
Propyl butyrate	3.79	4.27	-0.48
Propylene	0.92	1.45	-0.53
Propylenecarbonate	4.81	3.73	1.08
Propyleneglycol-1-monomethylether-2-acetate	4.16	3.91	0.25
Propyne	1.15	1.52	-0.37
Proquinazid	10.43	10.72	-0.29
Prosulfocarb	8.74	9.04	-0.30
Prothiofos	8.78	8.54	0.24
Pseudococaine	10.58	10.08	0.50
p-Toluidine	5.31	5.79	-0.48
Pulegone	5.87	5.53	0.34
Pyraclofos	11.32	11.27	0.05
Pyrasulfotole	10.47	10.55	-0.08
Pyrene	8.83	9.42	-0.59
Pyridalyl	12.64	11.76	0.88
Pyridaphenthion	10.93	11.06	-0.13
Pyridine	3.91	3.99	-0.08
Pyrifenox	9.33	9.16	0.17
Pyriktalid	11.11	10.64	0.47
Pyrimethanil	8.43	8.23	0.20
Pyriminobac-methyl	9.53	10.32	-0.79
Pyroquilon	8.42	8.01	0.41
Pyrrole	3.77	4.42	-0.65
Pyrrolidine	4.07	3.65	0.42
Pyruvic acid	5.16	5.59	-0.43
Quinalphos	9.8	9.8	0.00
Quinoclamine	9.39	9.68	-0.29
Quinoline	6.06	6.29	-0.23
Quinoxifen	9.37	10.17	-0.80
Radox	6.56	7.01	-0.45
Resmethrin	11.19	10.35	0.84
Sabinene	4.39	4.38	0.01
Salicylic acid	7.44	7.76	-0.32
s-Butylacetate	3.32	3.59	-0.27
s-Butylbenzene	4.2	4.43	-0.23
Sebuthylazine	8.74	9.32	-0.58
Secbumeton	8.99	9.6	-0.61
Sethoxydim	11.21	11.35	-0.14
Siduron	12.13	11.42	0.71
Simazine	8.81	8.79	0.02

Simeconazole	10	9.99	0.01
Simeton	9.35	9.07	0.28
Simetryn	9.86	9.67	0.19
Sorbic acid	7.11	5.87	1.24
Sorbitol	14.28	14.46	-0.18
Spiroxamine	8.57	8.78	-0.21
Stirofos	10.13	10.42	-0.29
s-trans-1,3-Butadiene	1.62	1.64	-0.02
Styrene	3.93	3.71	0.22
Styrene oxide	4.54	4.77	-0.23
Sulfometuron	15.41	15.66	-0.25
Sulprofos	9.42	8.75	0.67
t-Butylacetate	3.26	3.34	-0.08
t-Butylbenzene	4.18	4.02	0.16
Tebuconazole	11.41	10.82	0.59
Tebupirimfos	8.72	8.61	0.11
Tebuthiuron	9.47	9.32	0.15
Tedion	8.54	8.71	-0.17
Teflubenzuron	11.14	12.12	-0.98
Teproloxydim	10.28	11.35	-1.07
Terbacil	9.76	9.05	0.71
Terbufos	7.97	8.38	-0.41
Terbumeton	9.35	9.12	0.23
Terbutylazine	8.92	8.84	0.08
Terbutryne	9.9	9.72	0.18
Terpinolene	4.59	4.87	-0.28
Tetrabromobisphenol A	14.83	15.15	-0.32
Tetrachlorocatechol	9.09	10.42	-1.33
Tetrachloroethylene	3.48	3.74	-0.26
Tetrachloroveratrole	7.31	6.76	0.55
Tetraconazole	9.97	9.55	0.42
Tetradecane	6.11	5.78	0.33
Tetradisul	10.09	9.4	0.69
Tetrahydrofuran	2.86	2.82	0.04
Tetrahydropyran	3.22	3.14	0.08
Tetramethylene glycol	6.65	6.28	0.37
Tetramethylsilane	1.81	1.81	0.00
Thenylchlor	9.85	10.07	-0.22
Thi fluzamide	13.4	12.45	0.95
Thimet	7.54	7.68	-0.14
Thioanisoie	4.71	4.73	-0.02
Thiobencarb	8.92	8.78	0.14

Thiofanocarb	8.98	8.64	0.34
Thiophene	2.91	2.8	0.11
Thiophos	8.23	7.97	0.26
Thioxamyl	9.8	10.19	-0.39
TNT	7.53	7.99	-0.46
Tolclofos-methyl	7.83	7.56	0.27
Tonalide	8.24	8.03	0.21
Tralkoxydim	11.89	12.18	-0.29
trans-1,2-Cycloheptyl dinitrate	6.7	6.58	0.12
trans-1,2-Cyclohexyl dinitrate	5.66	6.26	-0.60
trans-1,2-Dichloroethylene	2.73	2.34	0.39
trans-1,3-Cyclohexyl dinitrate	6.05	6.26	-0.21
trans-1,3-Dichloropropene	3.28	2.95	0.33
trans-1,4-Dichloro-2-butene	4.15	3.56	0.59
trans-2,5-Dimethyltetrahydrofuran	3.41	3.18	0.23
trans-2-Butene	1.42	1.88	-0.46
trans-2-Methylcyclohexanol	5.22	5.29	-0.07
trans-2-Octenal	4.53	4.79	-0.26
trans-2-Octene	3.16	3.48	-0.32
trans-4-Methylcyclohexanol	5.47	5.29	0.18
trans-Decalin	4.2	4.47	-0.27
Transfluthrin	8.36	7.76	0.60
trans-Geraniol	6.43	6.34	0.09
trans-Nonachlor	9.29	9.6	-0.31
trans-Stilbene	7.48	6.4	1.08
Traseolide	8.18	8.26	-0.08
Tri-2-butoxyethyl phosphate	10.9	11.3	-0.40
Triadimenol	11.13	11.78	-0.65
Triallate	7.95	7.8	0.15
Triallylamine	4.53	4.2	0.33
Triasulfuron	13.47	12.57	0.90
Triazophos	9.59	9.41	0.18
Triazothion	9.59	9.91	-0.32
Tributyl phosphate	8.03	8.15	-0.12
Trichlopyr	9.48	9.28	0.20
Trichloroacetic acid	7.36	6.2	1.16
Trichloroethylene	3	3.04	-0.04
Trichloronate	8.42	8.42	0.00
Trichlorosyringol	8.69	8.51	0.18
Tricyclene	3.87	4	-0.13
Tridecane	5.34	5.4	-0.06
Tridecylamine	8.24	7.85	0.39

Tridiphan	7.09	8.27	-1.18
Triethyl phosphate	5.21	5.57	-0.36
Triethylamine	3.45	3.54	-0.09
Trifloxystrobin	10.46	10.07	0.39
Triflumuron	11.31	12.38	-1.07
Trihexyl phosphate	11.6	10.73	0.87
Tri-m-cresylphosphate	11.06	11.21	-0.15
Trimethyl phosphate	5.3	4.67	0.63
Trimethylacetic acid	5.29	5.1	0.19
Trimethylamine	2.36	2.28	0.08
Trimethyleneglycol dinitrate	5.08	5.13	-0.05
Trimethylethylene	1.78	2.24	-0.46
tri-n-Amylphosphate	9.31	9.44	-0.13
Tri-o-cresylphosphate	10.7	11.21	-0.51
Tri-p-cresyl phosphate	11.3	11.21	0.09
Triphenyl phosphate	10.09	9.98	0.11
Tripropyl phosphate	6.2	6.86	-0.66
Tripropylamine	4.34	4.83	-0.49
Tris(2-chloroethyl) phosphate	7.85	7.91	-0.06
Tris(2-ethylhexyl) phosphate	11.9	12.44	-0.54
Tris(2-isopropylphenyl) phosphate	11.78	12.92	-1.14
Tris-BP	13.5	12.86	0.64
Tycor	8.32	8.83	-0.51
Undecane	4.56	4.64	-0.08
Veratrole	4.93	4.36	0.57
Vernolate	6.8	7.06	-0.26
Vinclozolin	8.69	7.8	0.89
Vinyl acetate	2.33	2.49	-0.16
Vinylidenechloride	2.34	2.41	-0.07
Vitavax	9.81	9.58	0.23