

Molecule name	logP exp	logP calc	Diff
(2-Bromoethyl)benzene	3.09	3.15	-0.06
(2-Pyridyl)acetamide	-0.65	0.2	-0.85
(3-Bromopropyl)benzene	3.72	3.59	0.13
(3-Chloropropyl)benzene	3.55	3.51	0.04
(9Z)-Octadecenoic acid	7.64	6.79	0.85
(Bromomethyl)benzene	2.92	2.71	0.21
(Chloromethyl)benzene	2.3	2.63	-0.33
(E) 4-Decenal	4.05	3.39	0.66
(Ethylthio)benzene	3.2	2.98	0.22
(L)-Alanine	-2.83	-2.92	0.09
(L)-Cysteine	-2.49	-2.87	0.38
(L)-Histidine	-2.52	-3.32	0.80
(L)-Methionine	-1.87	-2.03	0.16
(S)-(+)-Nirvanol	1.53	1.56	-0.03
(Trichloromethyl)benzene	2.92	3.9	-0.98
(Z) 7-Decenal	3.52	3.39	0.13
1 1-Bis(methylthio)-2-nitroethylene	1.69	1.68	0.01
1-(2,4,5-Trichlorophenylhydrazono)-1-cyanoacetic acid ethylester	5.21	5.06	0.15
1-(2,4,5-Trichlorophenylhydrazono)-1-cyanoacetic acid methylester	5.15	4.63	0.52
1-(2,4-Dinitrophenylhydrazono)-1-cyanoacetic acid ethylester	4.14	3.72	0.42
1-(2,4-Dinitrophenylhydrazono)-1-cyanoacetone	3.41	3.22	0.19
1-(2,6-Cl2-4-CF3-phenylhydrazono)-1-cyanoacetic acid methylester	4.36	5.03	-0.67
1-(2-CF3-phenylhydrazono)-1-cyanoacetic acid methylester	3.72	3.97	-0.25
1-(2-Chlorophenylhydrazono)-1-cyanoacetone	4.01	3.5	0.51
1-(2-Cl-5-CF3-phenylhydrazono)-1-cyanoacetic acid methylester	4.42	4.5	-0.08
1-(2-Cl-5-CF3-phenylhydrazono)-1-cyanoacetone	5.08	4.43	0.65
1-(2-Hydroxyphenyl)-1-propanone	2.54	2.26	0.28
1-(2-Methylsulfonyl-4-nitrophenylhydrazono)-1-cyanoacetic acid ethylester	3.21	2.84	0.37
1-(2-NO2-5-CF3-phenylhydrazono)-1-cyanoacetic acid methylester	3.44	4.35	-0.91
1-(2-Pyridinyl)ethanone	0.83	0.4	0.43
1-(3,4,5-Trichlorophenylhydrazono)-1-cyanoacetic acid ethylester	5.03	5.06	-0.03
1-(3,4,5-Trichlorophenylhydrazono)-1-cyanoacetic acid methylester	5.22	4.63	0.59
1-(3,4-Dichlorophenylhydrazono)-1-cyanoacetic acid ethylester	4.66	4.53	0.13
1-(3,4-Dichlorophenylhydrazono)-1-cyanoacetone	4.56	4.03	0.53
1-(3,5-Dichlorophenylhydrazono)-1-cyanoacetic acid ethylester	3.82	4.53	-0.71
1-(3,5-Dichlorophenylhydrazono)-1-cyanoacetic acid methylester	4.5	4.1	0.40
1-(3,5-Dichlorophenylhydrazono)-1-cyanoacetone	4.68	4.03	0.65
1-(3-CF3-phenylhydrazono)-1-cyanoacetic acid methylester	3.78	3.97	-0.19
1-(3-Chlorophenylhydrazono)-1-cyanoacetic acid methylester	3.56	3.57	-0.01
1-(3-Chlorophenylhydrazono)-1-cyanoacetone	3.91	3.5	0.41

1-(3-Cl-phenylhydrazono)-1-cyanoacetic acid ethylester	3.94	4	-0.06
1-(4-Carboxybutyl)benzotriazole	0.93	1.96	-1.03
1-(4-CF <sub>3</sub> SO <sub>2</sub> -phenylhydrazono)-1-cyanoacetic acid methylester	4.22	3.41	0.81
1-(4-CF <sub>3</sub> S-phenylhydrazono)-1-cyanoacetic acid methylester	4.27	4.89	-0.62
1-(4-Chlorophenylhydrazono)-1-cyanoacetone	4.13	3.5	0.63
1-(4-Cl-2-CF <sub>3</sub> -phenylhydrazono)-1-cyanoacetic acid methylester	4.66	4.5	0.16
1-(4-Cl-2-CH <sub>3</sub> -phenylhydrazono)-1-cyanoacetic acid methylester	4.28	3.91	0.37
1-(4-trifluoromethylthiophenylhydrazono)-1-cyanoacetone	5.04	4.82	0.22
1-(Chloromethyl)-2-fluorobenzene	2.67	2.65	0.02
1,1,1,2-Tetrachloroethane	2.62	2.66	-0.04
1,1,1,3,3,3-Hexafluoro-2-methoxypropane	2.91	2.35	0.56
1,1,1,3,3,3-Hexafluoro-2-phenyl-2-propanol	3.41	3.1	0.31
1,1,1-Trifluoro-2-propanol	0.71	1	-0.29
1,1,2,2-Tetrachloroethane	2.39	2.59	-0.20
1,1,2-Trichloroethane	1.89	1.99	-0.10
1,10-Decyl dinitrate	5.56	4.95	0.61
1,13-Tridecanedioic acid	3.99	3.72	0.27
1,1-Bis(methylthio)ethylene	2.04	2.26	-0.22
1,1-Dichloroacetone	0.97	1.07	-0.10
1,1-Dichloroethane	1.79	1.93	-0.14
1,1-Dicyano-2,2-bis(methylthio)ethylene	1.16	0.99	0.17
1,1-Diethoxyethane	0.84	1.44	-0.60
1,1-Dimethyl-3-phenylurea	0.98	1.52	-0.54
1,1-Dimethylpropargylamine	0.64	0.34	0.30
1,2,3,4,5,6,8-Heptachloronaphthalene	7.46	6.94	0.52
1,2,3,4,5,7-Hexachloronaphthalene	7.58	6.41	1.17
1,2,3,4,6,7,8-Heptachlorodibenzofuran	7.92	7.71	0.21
1,2,3,4,6,7-Hexachloronaphthalene	6.77	6.41	0.36
1,2,3,4,6-Pentachloronaphthalene	7	5.88	1.12
1,2,3,4,7-Pentachlorodibenzofuran	6.53	6.65	-0.12
1,2,3,4,7-Pentachlorodibenzo-p-dioxin	6.6	6.64	-0.04
1,2,3,4-Tetrachlorobenzene	4.64	4.35	0.29
1,2,3,4-Tetrachlorodibenzofuran	6.17	6.12	0.05
1,2,3,4-Tetrachlorodibenzo-p-dioxin	7.18	6.11	1.07
1,2,3,4-Tetrachloronaphthalene	5.9	5.35	0.55
1,2,3,4-Tetrahydronaphthalene	3.49	3.91	-0.42
1,2,3,4-Tetrahydroquinoline	2.29	2.39	-0.10
1,2,3,5,7,8-Hexachloronaphthalene	7.33	6.41	0.92
1,2,3,5,7-Pentachloronaphthalene	6.87	5.88	0.99
1,2,3,5,8-Pentachloronaphthalene	6.46	5.88	0.58
1,2,3,5-Tetrachlorobenzene	4.66	4.35	0.31
1,2,3,5-Tetrachloronaphthalene	5.78	5.35	0.43

1,2,3,5-Tetramethylbenzene	4.04	3.79	0.25
1,2,3,7,8-Pentachlorodibenzofuran	6.79	6.65	0.14
1,2,3,7,8-Pentachlorodibenzo-p-dioxin	6.64	6.64	0.00
1,2,3,7-Tetrachlorodibenzofuran	6.04	6.12	-0.08
1,2,3-Propanetricarboxylic acid	-1.72	-1.65	-0.07
1,2,3-Propanetriol	-1.79	-1.73	-0.06
1,2,3-Tribromobenzene	4.98	4.18	0.80
1,2,3-Trichlorobenzene	4.14	3.82	0.32
1,2,3-Trichloropropane	1.98	2.08	-0.10
1,2,3-Triiodobenzene	5.86	5.26	0.60
1,2,3-Trimethoxybenzene	1.53	2.02	-0.49
1,2,4,5-Tetrabromobenzene	5.13	4.83	0.30
1,2,4,5-Tetrachlorobenzene	4.63	4.35	0.28
1,2,4,5-Tetrafluorobenzene	2.44	2.31	0.13
1,2,4,5-Tetramethylbenzene	4	3.79	0.21
1,2,4,6,7,9-Hexachlorodibenzo-p-dioxin	7.85	7.17	0.68
1,2,4,7,8-Pentachlorodibenzofuran	6.26	6.65	-0.39
1,2,4,7,8-Pentachlorodibenzo-p-dioxin	6.64	6.64	0.00
1,2,4-Tribromobenzene	4.32	4.18	0.14
1,2,4-Trichlorobenzene	4.02	3.82	0.20
1,2,4-Trichlorodibenzo-p-dioxin	6.34	5.58	0.76
1,2,4-Trifluorobenzene	2.41	2.29	0.12
1,2,4-Triiodobenzene	5.85	5.26	0.59
1,2,4-Trimethylbenzene	3.7	3.43	0.27
1,2,7,8-Tetrachlorodibenzofuran	6.23	6.12	0.11
1,2,7,8-Tetrachlorodibenzo-p-dioxin	6.38	6.11	0.27
1,2-Benzenedicarboxylic acid, di-2-propenyl ester	3.23	2.63	0.60
1,2-Bis(dimethylamino)ethane	0.3	0.07	0.23
1,2-Diaminobenzene	0.15	0.41	-0.26
1,2-Dibromobenzene	3.64	3.53	0.11
1,2-Dibromoethane	1.96	1.55	0.41
1,2-Dibromohexane	3.85	3.54	0.31
1,2-Dichlorobenzene	3.38	3.29	0.09
1,2-Dichloronaphthalene	4.66	4.29	0.37
1,2-Difluorobenzene	2.37	2.27	0.10
1,2-Dihydroxybenzene	0.88	1.43	-0.55
1,2-Dimethyl-3-nitrobenzene	2.83	2.78	0.05
1,2-Dimethyl-4-nitrobenzene	2.91	2.78	0.13
1,2-Dimethylbenzene	3.12	3.07	0.05
1,2-Dimethylindole	2.82	3.13	-0.31
1,2-Dimethylnaphthalene	4.31	4.15	0.16
1,2-Dimethylpropylamine	1.1	1	0.10

1,2-Dinitrobenzene	1.69	1.97	-0.28
1,2-Diphenylethane	4.79	5.03	-0.24
1,2-Diphenylhydrazine	2.94	3.03	-0.09
1,2-Ethanediol	-1.36	-1.13	-0.23
1,2-Ethanediol dinitrate	1.37	1.43	-0.06
1,3,5,7-Tetrachloronaphthalene	6.19	5.35	0.84
1,3,5,8-Tetrachloronaphthalene	5.81	5.35	0.46
1,3,5-Cycloheptatriene	2.63	2.75	-0.12
1,3,5-Tribromobenzene	4.51	4.18	0.33
1,3,5-Trichlorobenzene	4.19	3.82	0.37
1,3,5-Trihydroxybenzene	0.16	1.03	-0.87
1,3,5-Triiodobenzene	5.85	5.26	0.59
1,3,5-Trimethylbenzene	3.42	3.43	-0.01
1,3,5-Trinitrobenzene	1.18	1.84	-0.66
1,3,6,8-Tetrachlorodibenzofuran	6.37	6.12	0.25
1,3,6,8-Tetrachlorodibenzo-p-dioxin	6.29	6.11	0.18
1,3,7,8-Tetrachlorodibenzofuran	6.39	6.12	0.27
1,3,7,9-Tetrachlorodibenzofuran	6.39	6.12	0.27
1,3,7,9-Tetrachlorodibenzo-p-dioxin	6.39	6.11	0.28
1,3,7-Trichlorodibenzo-p-dioxin	6.31	5.58	0.73
1,3,7-Trichloronaphthalene	5.35	4.82	0.53
1,3-Benzodioxole	2.08	2.16	-0.08
1,3-Bis(trifluoromethyl)benzene	3.83	4.09	-0.26
1,3-Butyl dinitrate	2.15	2.34	-0.19
1,3-Cyclohexadiene	2.47	2.55	-0.08
1,3-Cyclohexanedione	-0.45	0.49	-0.94
1,3-Diamino-2-propanol	-2.05	-2.43	0.38
1,3-Dibromobenzene	3.75	3.53	0.22
1,3-Dichloro-2-propanol	0.2	0.53	-0.33
1,3-Dichloro-4-fluorobenzene	2.91	3.31	-0.40
1,3-Dichloroacetone	0.02	0.53	-0.51
1,3-Dichlorobenzene	3.53	3.29	0.24
1,3-Dichloropropane	2	1.83	0.17
1,3-Difluorobenzene	2.21	2.27	-0.06
1,3-Dihydroxybenzene	0.8	1.43	-0.63
1,3-Dimethoxybenzene	2.21	2.09	0.12
1,3-Dimethylbenzene	3.2	3.07	0.13
1,3-Dimethylimidazolium chloride	1.9	2.16	-0.26
1,3-Dimethylimidazolium methosulfate	-0.41	-0.47	0.06
1,3-Dimethylnaphthalene	4.42	4.15	0.27
1,3-Dimethyluracil	0	-0.89	0.89
1,3-Dinitrobenzene	1.49	1.97	-0.48

1,3-Dithiolane	1.58	1.29	0.29
1,3-Propanediamine	-1.43	-1.13	-0.30
1,4,5-Trimethylnaphthalene	4.9	4.51	0.39
1,4-Benzoquinone	0.2	-0.03	0.23
1,4-Butyl dinitrate	2.17	2.31	-0.14
1,4-Cyclohexadiene	2.3	2.69	-0.39
1,4-Cyclohexanedione	-0.52	0.49	-1.01
1,4-Diaminobenzene	-0.3	0.41	-0.71
1,4-Dibromo-2,3-butanedione	-0.86	-0.17	-0.69
1,4-Dibromo-2-butene	2.03	2.03	0.00
1,4-Dibromobenzene	3.79	3.53	0.26
1,4-Dichlorobenzene	3.44	3.29	0.15
1,4-Dichlorobutane	2.81	2.27	0.54
1,4-Dichloronaphthalene	4.66	4.29	0.37
1,4-Difluorobenzene	2.13	2.27	-0.14
1,4-Dihydroxybenzene	0.59	1.43	-0.84
1,4-Diiodobenzene	4.11	4.25	-0.14
1,4-Dimethoxy-2,3,5,6-tetrachlorocyclohexane	3.15	2.45	0.70
1,4-Dimethylbenzene	3.15	3.07	0.08
1,4-Dimethylnaphthalene	4.37	4.15	0.22
1,4-Dimethylquinoxalin-2,3-dione	0.08	-0.03	0.11
1,4-Dinitrobenzene	1.49	1.97	-0.48
1,4-Dioxane	-0.27	-0.39	0.12
1,4-Dioxatetralin	2.01	1.99	0.02
1,4-Di-t-butylbenzene	5.63	5.35	0.28
1,4-Naphthoquinone	1.78	1.13	0.65
1,4-Pentadiene	2.48	2.25	0.23
1,4-Pentyl dinitrate	2.88	2.78	0.10
1,5-Cyclooctadiene	3.55	3.33	0.22
1,5-Dichloropentane	3.3	2.71	0.59
1,5-Dimethylnaphthalene	4.38	4.15	0.23
1,5-Hexadiene	2.45	2.71	-0.26
1,5-Hexyl dinitrate	3.25	3.22	0.03
1,5-Pentanediol	0.3	0.19	0.11
1,5-Pentyl dinitrate	2.64	2.75	-0.11
1,6-Dibromohexane	3.57	3.31	0.26
1,6-Hexanedioic acid	0.08	0.64	-0.56
1,6-Hexanedithiol	2.71	3.13	-0.42
1,6-Hexyl dinitrate	3.19	3.19	0.00
1,7-Dimethylnaphthalene	4.44	4.15	0.29
1,7-Heptyl dinitrate	3.81	3.63	0.18
1,7-Phenanthroline	2.51	2.33	0.18

1,8-Dichloronaphthalene	4.19	4.29	-0.10
1,8-Dimethylnaphthalene	4.26	4.15	0.11
1,8-Octanedithiol	3.77	4.01	-0.24
1,8-Octyl dinitrate	4.4	4.07	0.33
11-Deoxycorticosterone	2.88	3.41	-0.53
17a-Hydroxyprogesterone	3.17	3.37	-0.20
17a-Methyltestosterone	3.36	4.23	-0.87
1-Acetoxy-2,3,4,5,6-pentachlorocyclohexane	3.4	3.45	-0.05
1-Adamantanol	2.14	2.12	0.02
1-Amino-3-methoxypropane	-1.02	-0.28	-0.74
1-Aminoacridine	2.47	2.77	-0.30
1-Aminoadamantane	2.44	2.18	0.26
1-Azabicyclo[2.2.2]octane	1.2	1.47	-0.27
1-Benzyl-3-methylimidazolium chloride	2.99	4.01	-1.02
1-Benzyl-3-methylimidazolium tetrafluoroborate	4.8	5.62	-0.82
1-Benzylbenzimidazole	3.24	3	0.24
1-Benzylimidazole	1.6	1.06	0.54
1-Bromo-2-propanol	0.28	0.55	-0.27
1-Bromo-3-chloropropane	2.18	1.91	0.27
1-Bromobutane	2.75	2.29	0.46
1-Bromooctane	4.89	4.05	0.84
1-Bromopentane	3.37	2.73	0.64
1-Bromopinacolone	1.28	1.63	-0.35
1-Bromopropane	2.1	1.85	0.25
1-Butanethiol	2.28	2.2	0.08
1-Butanol	0.79	0.82	-0.03
1-Butene	1.59	2.01	-0.42
1-Butyl-3-methylimidazolium bromide	3.59	3.59	0.00
1-Butyl-3-methylimidazolium chloride	3.25	3.59	-0.34
1-Butyl-3-methylimidazolium iodide	3.79	3.59	0.20
1-Butyl-3-methylimidazolium methosulfate	0.94	0.96	-0.02
1-Butyl-3-methylimidazolium tetrafluoroborate	5.06	5.2	-0.14
1-Butyl-3-methylpyridinium tetrafluoroborate	4.77	4.78	-0.01
1-Butyl-4-methylpyridinium tetrafluoroborate	4.98	4.78	0.20
1-Butylamine	0.97	0.73	0.24
1-Butylpyridinium chloride	2.78	2.83	-0.05
1-Butylpyridinium tetrafluoroborate	4.59	4.44	0.15
1-Butyne	1.44	1.45	-0.01
1-Chloro-2-propanol	0.14	0.47	-0.33
1-Chlorobutane	2.55	2.21	0.34
1-Chlorodibenzo-p-dioxin	5.05	4.52	0.53
1-Chloroheptane	4.15	3.53	0.62

1-Chloronaphthalene	4.24	3.76	0.48
1-Chloropentane	2.73	2.65	0.08
1-Chloropropane	2.04	1.77	0.27
1-Decyl-3-methylimidazolium bromide	7	6.23	0.77
1-Decyl-3-methylimidazolium tetrafluoroborate	8.48	7.84	0.64
1-Dimethylamino-2-propyne	-0.01	0.33	-0.34
1-Dodecyl-3-methylimidazolium bromide	7	7.11	-0.11
1-Ethoxy-butane	2.03	2.01	0.02
1-Ethyl-1-hydroxyurea	-0.1	-0.02	-0.08
1-Ethyl-3-methylimidazolium bromide	2.66	2.71	-0.05
1-Ethyl-3-methylimidazolium chloride	2.33	2.71	-0.38
1-Ethyl-3-methylimidazolium ethosulfate	0.44	0.51	-0.07
1-Ethyl-3-methylimidazolium tetrafluoroborate	4.14	4.32	-0.18
1-Ethyl-naphthalene	4.39	4.25	0.14
1-Fluoropentane	2.33	2.03	0.30
1-Heptanethiol	3.82	3.52	0.30
1-Heptanol	2.57	2.14	0.43
1-Heptene	3.99	3.39	0.60
1-Heptyn-3-ol	1.73	1.39	0.34
1-Hexanol	2.03	1.7	0.33
1-Hexen-3-ol	1.18	1.51	-0.33
1-Hexen-5-one	1.02	1.51	-0.49
1-Hexene	3.39	2.93	0.46
1-Hexyl-3-methylimidazolium bromide	4.73	4.47	0.26
1-Hexyl-3-methylimidazolium chloride	4.39	4.47	-0.08
1-Hexyl-3-methylimidazolium iodide	4.93	4.47	0.46
1-Hexyl-3-methylimidazolium tetrafluoroborate	6.2	6.08	0.12
1-Hexyn-3-ol	1.2	0.95	0.25
1-Hexyne	2.73	2.37	0.36
1H-Indazole	1.82	2.6	-0.78
1H-Indene-1,3(2H)-dione	0.61	1.09	-0.48
1H-Purine	-0.37	-0.28	-0.09
1H-Pyrazole	0.13	1.05	-0.92
1-Hydroxy-2,3,4,5,6-pentachlorocyclohexane	2.54	2.48	0.06
1-Iodobutane	3.06	2.96	0.10
1-Iodoheptane	4.7	4.28	0.42
1-Iodopentane	3.56	3.4	0.16
1-Isopropylbenzotriazole	1.98	2.19	-0.21
1-Methoxy-2-propanamine	-0.36	-0.29	-0.07
1-Methoxy-3-phenylpropane	2.7	2.88	-0.18
1-Methyl-1-hydroxypentachlorocyclohexane	2.94	2.69	0.25
1-Methyl-1-hydroxyurea	-0.46	-0.57	0.11

1-Methyl-4-isopropylcyclohexene	4.57	4.16	0.41
1-Methyl-4-phenylquinazolin-2-one	1.79	2.53	-0.74
1-Methylbenzotriazole	1.13	1.21	-0.08
1-Methylfluorene	4.97	5.07	-0.10
1-Methylisatin	0.58	0.31	0.27
1-Methylnaphthalene	3.87	3.79	0.08
1-Methylphenanthrene	5.08	4.87	0.21
1-Methyluracil	-1.2	-0.78	-0.42
1-Naphthalenecarboxylic acid	3.1	2.45	0.65
1-Naphthol	2.84	2.83	0.01
1-Naphthyl acetate	2.78	3.18	-0.40
1-Naphthylamine	2.25	2.32	-0.07
1-Naphthylisothiocyanate	4.34	4.18	0.16
1-Naphthylmethylisothiocyanate	4.42	4.53	-0.11
1-Nitrobutane	1.47	1.29	0.18
1-Nitronaphthalene	3.19	3.1	0.09
1-Nitropentane	2.01	1.73	0.28
1-Nitropropane	0.65	0.85	-0.20
1-Nonanol	3.77	3.02	0.75
1-Nonene	5.15	4.31	0.84
1-Octanol	3	2.58	0.42
1-Octyl-3-methylimidazolium bromide	5.87	5.35	0.52
1-Octyl-3-methylimidazolium chloride	5.53	5.35	0.18
1-Octyl-3-methylimidazolium tetrafluoroborate	7.34	6.96	0.38
1-Pentanethiol	2.74	2.64	0.10
1-Pentanol	1.4	1.26	0.14
1-Penten-3-ol	0.65	1.07	-0.42
1-Pentylbenzimidazole	3.63	3.02	0.61
1-Pentylbenzotriazole	3.22	3.08	0.14
1-Pentyn-3-ol	0.67	0.51	0.16
1-Pentyne	1.98	1.91	0.07
1-Phenethylisothiocyanate	3.46	3.96	-0.50
1-Phenyl-1,3-butanedione (enol form)	2.52	2.38	0.14
1-Phenyl-1-propanone	2.19	2.15	0.04
1-Phenyl-2-acetamidocyclopropane	1.43	2	-0.57
1-Phenyl-2-butanol	2.02	2.59	-0.57
1-Phenyl-2-nitropropene	2.52	2.52	0.00
1-Phenylhydrazono-1-cyanoacetic acid methylester	2.59	3.04	-0.45
1-Phenyltetrazole	1.09	0.8	0.29
1-Propanethiol	1.81	1.76	0.05
1-Propanol	0.34	0.38	-0.04
1-Propyl-3-methylimidazolium iodide	3.22	3.15	0.07

1-Propyl-3-methylimidazolium tetrafluoroborate	4.33	4.76	-0.43
1-Propylamine	0.48	0.29	0.19
1-Propylbenzotriazole	2.13	2.2	-0.07
1-Propylpyridinium chloride	2.21	2.39	-0.18
1-s-Butylbenzotriazole	2.31	2.48	-0.17
1-Undecanol	4.54	3.9	0.64
2-(2,4,6-Tribromophenoxy)ethanol	3.42	3.21	0.21
2-(2,4-Dichlorophenoxy)propanoic acid	3.43	3	0.43
2-(2-Pyridyl)ethanol	0.12	0.37	-0.25
2-(2-Pyridyl)ethylamine	0.08	0.28	-0.20
2-(3-Hydroxypropyl)benzimidazole	1.25	1.38	-0.13
2-(3-Pyridyl)ethanol	0.12	0.33	-0.21
2-(3-Pyridyl)ethylamine	0	0.24	-0.24
2-(4-Pyridyl)ethanol	0.1	0.33	-0.23
2-(6-Methoxynaphthalen-2-yl)propanoic acid	3.18	3.1	0.08
2-(Ethylamino)ethanol	-0.46	-0.52	0.06
2-(Hydroxymethyl)-1-methyl-5-nitroimidazole	-0.03	-0.46	0.43
2-(Methylthio)aniline	1.2	1.79	-0.59
2-(Methylthio)phenyl N-methylcarbamate	1.51	1.92	-0.41
2-(Methylthio)quinoxaline	2.79	2.3	0.49
2-(Phenoxymethyl)oxirane	1.6	1.96	-0.36
2-(Propylamino)ethanol	0.07	-0.08	0.15
2-(t-Butylamino)ethanol	0.41	0.31	0.10
2,2,2-Trichloroethanol	1.42	1.27	0.15
2,2,2-Trifluoroethanol	0.41	0.53	-0.12
2,2,2-Trifluoroethylacetate	1.18	1.5	-0.32
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	7.51	8.64	-1.13
2,2',3,3',4,4',5,5',6-Nonachlorodiphenyl ether	8.07	8.63	-0.56
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	7.65	8.11	-0.46
2,2',3,3',4,4',5,5'-Octachlorodiphenyl ether	7.78	8.1	-0.32
2,2',3,3',4,4',5,6,6'-Nonachlorobiphenyl	7.88	8.64	-0.76
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	7.43	8.11	-0.68
2,2',3,3',4,4',5-Heptachlorobiphenyl	6.96	7.58	-0.62
2,2',3,3',4,4',6-Heptachlorobiphenyl	7.21	8.11	-0.90
2,2',3,3',4,4',6-Heptachlorobiphenyl	6.68	7.58	-0.90
2,2',3,3',4,4'-Hexachlorobiphenyl	7.32	7.05	0.27
2,2',3,3',4,4'-Hexachlorodiphenyl ether	6.82	7.04	-0.22
2,2',3,3',4,5,5',6'-Octachlorobiphenyl	7.21	8.11	-0.90
2,2',3,3',4,5,5',6-Octachlorobiphenyl	7.43	8.11	-0.68
2,2',3,3',4,5,5'-Heptachlorobiphenyl	7.03	7.58	-0.55
2,2',3,3',4,5,6,6'-Octachlorobiphenyl	7.35	8.11	-0.76
2,2',3,3',4,5,6'-Heptachlorobiphenyl	6.73	7.58	-0.85

2,2',3,3',4,5',6-Heptachlorobiphenyl	6.92	7.58	-0.66
2,2',3,3',4,5'-Hexachlorobiphenyl	7.39	7.05	0.34
2,2',3,3',4,6,6'-Heptachlorobiphenyl	6.65	7.58	-0.93
2,2',3,3',4,6'-Hexachlorobiphenyl	7.04	7.05	-0.01
2,2',3,3',4,6-Hexachlorobiphenyl	6.82	7.05	-0.23
2,2',3,3',4-Pentabromodiphenyl ether	6.97	7.11	-0.14
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	7.73	8.11	-0.38
2,2',3,3',5,5',6-Heptachlorobiphenyl	6.85	7.58	-0.73
2,2',3,3',5,5'-Hexachlorobiphenyl	7.07	7.05	0.02
2,2',3,3',5,6,6'-Heptachlorobiphenyl	6.41	7.58	-1.17
2,2',3,3',5,6'-Hexachlorobiphenyl	7.15	7.05	0.10
2,2',3,3',5,6-Hexachlorobiphenyl	6.91	7.05	-0.14
2,2',3,3',6,6'-Hexachlorobiphenyl	7.12	7.05	0.07
2,2',3,3',6-Pentachlorobiphenyl	6.04	6.52	-0.48
2,2',3,3'-Tetrachlorobiphenyl	6.18	5.99	0.19
2,2',3,4,4',5,5',6-Octachlorobiphenyl	7.21	8.11	-0.90
2,2',3,4,4',5,5'-Heptachlorobiphenyl	6.89	7.58	-0.69
2,2',3,4,4',5,5'-Heptachlorodiphenyl ether	7.46	7.57	-0.11
2,2',3,4,4',5,6,6'-Octachlorobiphenyl	7.48	8.11	-0.63
2,2',3,4,4',5,6-Heptachlorobiphenyl	6.92	7.58	-0.66
2,2',3,4,4',5,6'-Heptachlorobiphenyl	6.92	7.58	-0.66
2,2',3,4,4',5,6-Heptachlorobiphenyl	7.13	7.58	-0.45
2,2',3,4,4',5,6'-Heptachlorodiphenyl ether	7.5	7.57	-0.07
2,2',3,4,4',5'-Hexachlorobiphenyl	7.25	7.05	0.20
2,2',3,4,4',5-Hexachlorobiphenyl	7.25	7.05	0.20
2,2',3,4,4',5'-Hexachlorodiphenyl ether	7.01	7.04	-0.03
2,2',3,4,4',5-Hexachlorodiphenyl ether	7.11	7.04	0.07
2,2',3,4,4',6,6'-Heptachlorobiphenyl	6.65	7.58	-0.93
2,2',3,4,4',6'-Hexachlorobiphenyl	6.97	7.05	-0.08
2,2',3,4,4',6-Hexachlorobiphenyl	6.95	7.05	-0.10
2,2',3,4,4',6'-Hexachlorodiphenyl ether	6.76	7.04	-0.28
2,2',3,4,4'-Pentabromodiphenyl ether	7.03	7.11	-0.08
2,2',3,4,4'-Pentachlorobiphenyl	6.61	6.52	0.09
2,2',3,4,4'-Pentachlorodiphenyl ether	6.28	6.51	-0.23
2,2',3,4,5,5',6-Heptachlorobiphenyl	6.99	7.58	-0.59
2,2',3,4',5,5',6-Heptachlorobiphenyl	6.84	7.58	-0.74
2,2',3,4,5,5'-Hexachlorobiphenyl	7.19	7.05	0.14
2,2',3,4',5,5'-Hexachlorobiphenyl	7.12	7.05	0.07
2,2',3,4',5,6,6'-Heptachlorobiphenyl	6.78	7.58	-0.80
2,2',3,4,5,6-Hexachlorobiphenyl	6.97	7.05	-0.08
2,2',3,4',5,6-Hexachlorobiphenyl	6.93	7.05	-0.12
2,2',3,4,5',6-Hexachlorobiphenyl	6.79	7.05	-0.26

2,2',3,4',5',6-Hexachlorobiphenyl	6.86	7.05	-0.19
2,2',3,4',5,6'-Hexachlorobiphenyl	6.87	7.05	-0.18
2,2',3,4',5-Pentachlorobiphenyl	6.32	6.52	-0.20
2,2',3,4,5'-Pentachlorobiphenyl	6.37	6.52	-0.15
2,2',3,4',5'-Pentachlorobiphenyl	6.67	6.52	0.15
2,2',3,4,6,6'-Hexachlorobiphenyl	6.71	7.05	-0.34
2,2',3,4',6,6'-Hexachlorobiphenyl	6.75	7.05	-0.30
2,2',3,4',6-Pentachlorobiphenyl	6.31	6.52	-0.21
2,2',3,4'-Tetrachlorobiphenyl	5.72	5.99	-0.27
2,2',3,4-Tetrachlorobiphenyl	6.11	5.99	0.12
2,2',3,5,5',6-Hexachlorobiphenyl	6.85	7.05	-0.20
2,2',3,5,5'-Pentachlorobiphenyl	6.97	6.52	0.45
2,2',3,5,6,6'-Hexachlorobiphenyl	6.51	7.05	-0.54
2,2',3,5,6-Pentachlorobiphenyl	6.06	6.52	-0.46
2,2',3,5',6-Pentachlorobiphenyl	5.92	6.52	-0.60
2,2',3,5'-Tetrachlorobiphenyl	5.81	5.99	-0.18
2,2',3-Trichlorobiphenyl	5.31	5.46	-0.15
2,2',4,4',5,5'-Hexabromodiphenyl ether	7.62	7.76	-0.14
2,2',4,4',5,5'-Hexachlorobiphenyl	7.5	7.05	0.45
2,2',4,4',5,5'-Hexachlorodiphenyl ether	6.72	7.04	-0.32
2,2',4,4',5,6'-Hexabromodiphenyl ether	7.39	7.76	-0.37
2,2',4,4',5,6'-Hexachlorobiphenyl	6.89	7.05	-0.16
2,2',4,4',5,6'-Hexachlorodiphenyl ether	6.49	7.04	-0.55
2,2',4,4',5-Pentabromodiphenyl ether	6.97	7.11	-0.14
2,2',4,4',5-Pentachlorobiphenyl	7.21	6.52	0.69
2,2',4,4',5-Pentachlorodiphenyl ether	6.38	6.51	-0.13
2,2',4,4',6,6'-Hexabromobiphenyl	7.2	7.77	-0.57
2,2',4,4',6,6'-Hexachlorobiphenyl	7.29	7.05	0.24
2,2',4,4',6-Pentabromodiphenyl ether	6.86	7.11	-0.25
2,2',4,4',6-Pentachlorobiphenyl	6.23	6.52	-0.29
2,2',4,4',6-Pentachlorodiphenyl ether	6.11	6.51	-0.40
2,2',4,4'-Tetrabromodiphenyl ether	6.39	6.46	-0.07
2,2',4,4'-Tetrachlorobiphenyl	6.29	5.99	0.30
2,2',4,4'-Tetrachlorodiphenyl ether	5.95	5.98	-0.03
2,2',4,5,5'-PCB	6.5	6.52	-0.02
2,2',4,5,5'-Pentabromobiphenyl	7.1	7.12	-0.02
2,2',4,5,5'-Pentachlorodiphenyl ether	6.22	6.51	-0.29
2,2',4,5',6-Pentachlorobiphenyl	6.11	6.52	-0.41
2,2',4,5'-Tetrachlorobiphenyl	6.38	5.99	0.39
2,2',4,6'-Tetrachlorobiphenyl	5.51	5.99	-0.48
2,2',4,6-Tetrachlorobiphenyl	5.75	5.99	-0.24
2,2',4-Tribromodiphenyl ether	5.58	5.81	-0.23

2,2',4-Trichlorobiphenyl	5.76	5.46	0.30
2,2',5,5'-Tetrabromobiphenyl	6.5	6.47	0.03
2,2',5,5'-Tetrachlorobiphenyl	6.09	5.99	0.10
2,2,5,5-Tetramethyltetrahydrofuran	2.06	2.13	-0.07
2,2',5,6'-Tetrachlorobiphenyl	5.98	5.99	-0.01
2,2',5-Trichlorobiphenyl	5.6	5.46	0.14
2,2',6,6'-Tetrachlorobiphenyl	5.94	5.99	-0.05
2,2,6,6-Tetramethyl-N-nitrosopiperidine	2.49	2.46	0.03
2,2',6-Trichlorobiphenyl	5.48	5.46	0.02
2,2'-Dichlorobiphenyl	4.97	4.93	0.04
2,2'-Dichlorodiisopropyl ether	2.48	2.19	0.29
2,2-Dichloroethanol	0.37	0.6	-0.23
2,2-Dichloropropionic acid	0.78	0.99	-0.21
2,2-Dimethylpropane	3.11	2.8	0.31
2,2-Diphenylpropionic acid	2.69	3.83	-1.14
2,3,3',4,4',5,5',6-Octachlorobiphenyl	7.62	8.11	-0.49
2',3,3',4,4',5,6-Heptabromodiphenyl ether	8.36	8.41	-0.05
2,3,3',4,4',5,6-Heptachlorobiphenyl	7.08	7.58	-0.50
2,3,3',4,4',5',6-Heptachlorobiphenyl	7.21	7.58	-0.37
2,3,3',4,4',5'-Hexabromodiphenyl ether	7.91	7.76	0.15
2,3,3',4,4',5-Hexabromodiphenyl ether	7.93	7.76	0.17
2,3,3',4,4',5'-Hexachlorobiphenyl	7.6	7.05	0.55
2,3,3',4,4',5-Hexachlorobiphenyl	7.57	7.05	0.52
2,3,3',4,4',6-Hexachlorobiphenyl	7.25	7.05	0.20
2,3,3',4,4'-Pentachlorobiphenyl	6.65	6.52	0.13
2,3,3',4,4'-Pentachlorodiphenyl ether	6.51	6.51	0.00
2,3,3',4,5,5',6-Heptachlorobiphenyl	7.21	7.58	-0.37
2,3,3',4',5,5',6-Heptachlorobiphenyl	7.21	7.58	-0.37
2,3,3',4,5,5'-Hexachlorobiphenyl	7.43	7.05	0.38
2,3,3',4',5,5'-Hexachlorobiphenyl	7.1	7.05	0.05
2,3,3',4,5,6-Hexachlorobiphenyl	7.3	7.05	0.25
2,3,3',4',5,6-Hexachlorobiphenyl	7.25	7.05	0.20
2,3,3',4,5',6-Hexachlorobiphenyl	7.1	7.05	0.05
2,3,3',4',5',6-Hexachlorobiphenyl	7.2	7.05	0.15
2,3,3',4,5-Pentachlorobiphenyl	6.92	6.52	0.40
2,3,3',4,6-Pentachlorobiphenyl	6.51	6.52	-0.01
2,3,3',4',6-Pentachlorobiphenyl	6.2	6.52	-0.32
2,3,3',4'-Tetrachlorobiphenyl	5.85	5.99	-0.14
2,3,3',5,5',6-Hexachlorobiphenyl	7.37	7.05	0.32
2,3,3',5,6-Pentachlorobiphenyl	6.41	6.52	-0.11
2,3,3',5',6-Pentachlorobiphenyl	6.45	6.52	-0.07
2,3,3',5'-Tetrachlorobiphenyl	6.17	5.99	0.18

2,3,3'-Trichlorobiphenyl	5.57	5.46	0.11
2,3',4,4',5,5'-Hexachlorobiphenyl	7.5	7.05	0.45
2,3',4,4',5,5'-Hexachlorodiphenyl ether	7.11	7.04	0.07
2,3,4,4',5,6-Hexachlorobiphenyl	7.31	7.05	0.26
2,3',4,4',5',6-Hexachlorobiphenyl	7.17	7.05	0.12
2,3',4,4',5'-Pentachlorobiphenyl	6.64	6.52	0.12
2,3',4,4',5-Pentachlorobiphenyl	6.57	6.52	0.05
2,3,4,4',6-Pentabromodiphenyl ether	6.97	7.11	-0.14
2,3,4,4',6-Pentachlorobiphenyl	6.44	6.52	-0.08
2,3',4,4',6-Pentachlorobiphenyl	6.4	6.52	-0.12
2,3',4,4'-Tetrabromodiphenyl ether	6.16	6.46	-0.30
2,3,4,4'-Tetrachlorobiphenyl	5.84	5.99	-0.15
2,3',4,4'-Tetrachlorobiphenyl	6.31	5.99	0.32
2,3',4,4'-Tetrachlorodiphenyl ether	6.13	5.98	0.15
2,3,4,5,6-Pentachlorobiphenyl	6.74	6.52	0.22
2,3',4,5',6-Pentachlorobiphenyl	6.42	6.52	-0.10
2,3,4',5,6-Pentachlorobiphenyl	6.39	6.52	-0.13
2,3,4,5-Tetrachloroaniline	4.27	3.44	0.83
2,3,4,5-Tetrachloroanisole	4.5	4.28	0.22
2,3',4',5'-Tetrachlorobiphenyl	5.98	5.99	-0.01
2,3,4,5-Tetrachlorobiphenyl	6.41	5.99	0.42
2,3',4,5-Tetrachlorobiphenyl	6.32	5.99	0.33
2,3,4',5-Tetrachlorobiphenyl	6.1	5.99	0.11
2,3',4',5-Tetrachlorobiphenyl	6.23	5.99	0.24
2,3,4,5-Tetrachloronitrobenzene	3.93	4.22	-0.29
2,3,4,5-Tetrachlorophenol	4.21	3.95	0.26
2,3',4,6-Tetrabromodiphenyl ether	6.16	6.46	-0.30
2,3,4',6-Tetrachlorobiphenyl	5.76	5.99	-0.23
2,3,4,6-Tetrachlorophenol	3.88	3.95	-0.07
2,3,4,7,8-Pentachlorodibenzofuran	6.92	6.65	0.27
2',3,4-Tribromodiphenyl ether	5.58	5.81	-0.23
2,3,4-Trichloroanisole	4.03	3.75	0.28
2,3',4'-Trichlorobiphenyl	5.87	5.46	0.41
2,3,4-Trichlorobiphenyl	5.86	5.46	0.40
2,3',4-Trichlorobiphenyl	5.54	5.46	0.08
2,3,4'-Trichlorobiphenyl	5.42	5.46	-0.04
2,3,4-Trichloronitrobenzene	3.61	3.69	-0.08
2,3,4-Trichlorophenol	3.61	3.42	0.19
2,3,5,6-Tetrachloroaniline	4.1	3.44	0.66
2,3,5,6-Tetrachloroanisole	4.4	4.28	0.12
2,3,5,6-Tetrachlorobiphenyl	5.96	5.99	-0.03
2,3,5,6-Tetrachloronitrobenzene	4.38	4.22	0.16

2,3,5,6-Tetrachlorophenol	3.88	3.95	-0.07
2,3,5,6-Tetrafluorothiophenol	1.76	2.28	-0.52
2,3,5,6-Tetramethyl-1,4-benzoquinone	2.23	1.61	0.62
2,3,5,6-Tetramethyl-4-hydroxyacetanilide	1.44	2.44	-1.00
2,3',5'-Trichlorobiphenyl	5.71	5.46	0.25
2,3',5-Trichlorobiphenyl	5.76	5.46	0.30
2,3,5-Trimethyl-4-hydroxyacetanilide	1.3	2.1	-0.80
2,3,6-Trichlorobiphenyl	5.67	5.46	0.21
2,3,6-Trimethyl-4-hydroxyacetanilide	1.24	2.1	-0.86
2,3,6-Trimethylnaphthalene	4.73	4.51	0.22
2,3,6-Trimethylphenol	2.67	2.85	-0.18
2,3,7,8-Tetrachlorodibenzofuran	6.53	6.12	0.41
2,3,7,8-Tetrachlorodibenzo-p-dioxin	6.53	6.11	0.42
2,3,7-Trichlorodibenzo-p-dioxin	6.46	5.58	0.88
2,3,8-Trichlorodibenzofuran	5.75	5.59	0.16
2,3-Butanedione	-1.34	-0.45	-0.89
2,3-Butyl dinitrate	2.36	2.37	-0.01
2,3-Butyleneglycol	-0.92	-0.19	-0.73
2,3-Dibromo-1-propanol	0.63	0.89	-0.26
2,3-Dichloroaniline	2.78	2.38	0.40
2,3-Dichloroanisole	3.24	3.22	0.02
2,3'-Dichlorobiphenyl	5.02	4.93	0.09
2,3-Dichlorobiphenyl	4.99	4.93	0.06
2,3-Dichlorodibenzofuran	5.43	5.06	0.37
2,3-Dichlorodibenzo-p-dioxin	5.8	5.05	0.75
2,3-Dichloronaphthalene	4.51	4.29	0.22
2,3-Dichloronitrobenzene	3.05	3.16	-0.11
2,3-Dichlorophenyl N-methylcarbamate	2.48	2.51	-0.03
2,3-Dichloropyridine	2.11	2.06	0.05
2,3-Dichlorothiophenol	2.44	3.26	-0.82
2,3-Dimethoxyamphetamine	1.49	1.88	-0.39
2,3-Dimethyl-4-hydroxyacetanilide	1.06	1.76	-0.70
2,3-Dimethylbutane	3.85	3.25	0.60
2,3-Dimethylphenyl N-methylcarbamate	1.95	2.13	-0.18
2,3-Xylenol	2.42	2.51	-0.09
2,3-Xylidine	1.81	2	-0.19
2,4,4',5-Tetrachlorobiphenyl	6.67	5.99	0.68
2,4,4',5-Tetrachlorodiphenyl ether	5.99	5.98	0.01
2,4,4',6-Tetrachlorobiphenyl	6.03	5.99	0.04
2,4,4'-Tribromodiphenyl ether	5.8	5.81	-0.01
2,4,4'-Trichlorobiphenyl	5.62	5.46	0.16
2,4,4'-Trichlorodiphenyl ether	5.53	5.45	0.08

2,4,5-T	3.13	3.06	0.07
2,4,5-Trichloroaniline	3.69	2.91	0.78
2,4,5-Trichlorobiphenyl	5.9	5.46	0.44
2,4',5-Trichlorobiphenyl	5.79	5.46	0.33
2,4,5-Trichlorodiphenyl ether	5.58	5.45	0.13
2,4',5-Trichlorodiphenyl ether	5.7	5.45	0.25
2,4,5-Trichloronitrobenzene	3.47	3.69	-0.22
2,4,5-Trichlorophenol	3.72	3.42	0.30
2,4,5-Trichlorotoluene	4.78	4.16	0.62
2,4,5-Trimethylphenyl N-methylcarbamate	2.52	2.47	0.05
2,4,5-Trioxoimidazolidine	-0.58	-1.52	0.94
2,4,6-Collidine	1.88	1.98	-0.10
2,4,6-Tribromobiphenyl	6.03	5.82	0.21
2,4,6-Tribromodiphenyl ether	5.58	5.81	-0.23
2,4',6-Tribromodiphenyl ether	5.59	5.81	-0.22
2,4,6-Tribromophenol	3.96	3.78	0.18
2,4,6-Tribromoresorcinol	4.37	3.38	0.99
2,4,6-Trichloroanisole	4.02	3.75	0.27
2,4,6-Trichlorobiphenyl	5.71	5.46	0.25
2,4',6-Trichlorobiphenyl	5.75	5.46	0.29
2,4,6-Trichlorodibenzofuran	5.69	5.59	0.10
2,4,6-Trichloronitrobenzene	3.69	3.69	0.00
2,4,6-Trichlorophenol	3.69	3.42	0.27
2,4,6-Trichloropurine	3.9	3.36	0.54
2,4,6-Trimethylphenyl isocyanate	3.21	3.31	-0.10
2,4,6-Trinitrophenol	1.33	1.95	-0.62
2,4,8-Trichlorodibenzofuran	5.69	5.59	0.10
2,4-Diaminobenzoic acid	-1.14	-1.69	0.55
2,4-Diaminophenol	-0.61	0.01	-0.62
2,4-Dibromo-2,4-dimethyl-3-pentanone	1.97	2.13	-0.16
2,4'-Dibromodiphenyl ether	5.03	5.16	-0.13
2,4-Dibromodiphenyl ether	5.03	5.16	-0.13
2,4-Dibromophenol	3.22	3.13	0.09
2,4-Dichloro-beta-nitrostyrene	3.26	3.27	-0.01
2,4'-Dichlorobiphenyl	5.1	4.93	0.17
2,4-Dichlorobiphenyl	5.15	4.93	0.22
2,4-Dichlorodiphenyl ether	4.93	4.92	0.01
2,4-Dichloronitrobenzene	3.09	3.16	-0.07
2,4-Dichlorophenol	3.06	2.89	0.17
2,4-Dichlorophenoxyacetic acid	2.58	2.53	0.05
2,4-Dichlorothiophenol	2.49	3.26	-0.77
2,4-Dichlorotoluene	4.24	3.63	0.61

2,4-Difluorophenol	1.9	1.87	0.03
2,4-Difluorothiophenol	1.34	2.24	-0.90
2,4-Dimethoxyamphetamine	1.75	1.88	-0.13
2,4-Dimethylthiophenol	3.77	2.88	0.89
2,4-Dinitroanisole	1.61	1.9	-0.29
2,4-Dinitrophenol	1.67	1.57	0.10
2,4-Dinitrotoluene	1.98	2.31	-0.33
2,4-Imidazolidinedione	-1.69	-1.01	-0.68
2,4-Nonanedione	1.65	1.75	-0.10
2,4-Octanedione	1.13	1.31	-0.18
2,4-Xylenol	2.35	2.51	-0.16
2,5-Diamino-1,3,4-thiadiazole	0.52	1.07	-0.55
2,5-Diaminonitrobenzene	0.53	0.79	-0.26
2,5-Dichloroaniline	2.75	2.38	0.37
2,5-Dichlorobiphenyl	5.16	4.93	0.23
2,5-Dichlorophenol	3.2	2.89	0.31
2,5-Dichlorophenyl N-methylcarbamate	2.44	2.51	-0.07
2,5-Dichloropyridine	2.4	2.06	0.34
2,5-Dichlorothiophenol	2.48	3.26	-0.78
2,5-Dihydrofuran	0.46	0.79	-0.33
2,5-Dihydroxybenzoic acid	1.18	1.16	0.02
2,5-Dimethoxyamphetamine	1.88	1.88	0.00
2,5-Dimethyl-4-hydroxyacetanilide	1.09	1.76	-0.67
2,5-Dimethylphenyl N-methylcarbamate	2.03	2.13	-0.10
2,5-Dimethylpyrazine	0.63	0.29	0.34
2,5-Dimethylthiophenol	3.92	2.88	1.04
2,5-Dinitrophenol	1.86	2.08	-0.22
2,5-Hexyl dinitrate	3.09	3.25	-0.16
2,5-Xylenol	2.34	2.51	-0.17
2,5-Xylidine	1.86	2	-0.14
2,6-Dibromo-4-nitrophenol	3.05	3	0.05
2,6-Dibromodiphenyl ether	5.03	5.16	-0.13
2,6-Dichloro-4-nitrophenol	2.94	2.76	0.18
2,6-Dichloroanisole	3.14	3.22	-0.08
2,6-Dichlorobenzonitrile	2.74	2.66	0.08
2,6-Dichlorobiphenyl	4.98	4.93	0.05
2,6-Dichlorodiphenyl ether	4.64	4.92	-0.28
2,6-Dichlorophenol	2.75	2.89	-0.14
2,6-Dichloropyridine	2.15	2.18	-0.03
2,6-Dichlorosyringaldehyde	2.52	2.09	0.43
2,6-Dichlorothiophenol	2.35	3.26	-0.91
2,6-Dichlorotoluene	4.29	3.63	0.66

2,6-Difluoropyridine	1.17	1.4	-0.23
2,6-Dihydroxybenzoic acid	2.2	1.67	0.53
2,6-Diisopropylaniline	3.18	3.44	-0.26
2,6-Diisopropylphenol	3.79	3.95	-0.16
2,6-Dimethoxyphenol	1.15	1.69	-0.54
2,6-Dimethyl-4-hydroxyacetanilide	0.8	1.76	-0.96
2,6-Dimethyl-N,N'-dinitrosopiperazine	0.08	-0.07	0.15
2,6-Dimethylnaphthalene	4.31	4.15	0.16
2,6-Dimethyl-N-nitrosomorpholine	0.32	0.2	0.12
2,6-Dimethyl-N-nitrosopiperidine	1.36	1.66	-0.30
2,6-Dimethylphenyl isocyanate	2.74	2.97	-0.23
2,6-Dimethylpyrazine	0.54	0.29	0.25
2,6-Dimethylthiophenol	4.02	2.88	1.14
2,6-Dinitroaniline	1.79	2.08	-0.29
2,6-Dinitrophenol	1.33	2.08	-0.75
2,6-Dinitrotoluene	2.1	2.31	-0.21
2,6-Diphenylpyridine	4.82	4.24	0.58
2,6-Di-s-butylphenol	4.36	4.83	-0.47
2,6-Di-t-butylpyridine	4.14	3.8	0.34
2,6-Lutidine	1.68	1.64	0.04
2,6-Xylenol	2.36	2.51	-0.15
2,7-Dichlorodibenzofuran	5.41	5.06	0.35
2,7-Dichlorodibenzo-p-dioxin	5.77	5.05	0.72
2,7-Dichloronaphthalene	4.56	4.29	0.27
2,8-Dichlorodibenzofuran	5.65	5.06	0.59
2,8-Dichlorodibenzo-p-dioxin	5.77	5.05	0.72
2,beta-Dinitrostyrene	1.8	2.08	-0.28
2,N,N-Trimethylaniline	2.85	2.26	0.59
2,5-Dichloronitrobenzene	3.03	3.16	-0.13
2-Acetamido-1,4-naphthoquinone	1.29	0.76	0.53
2-Acetamidopyridine	0.61	0.97	-0.36
2-Acetoxyanisole	1.38	2.11	-0.73
2-Acetylphenoxyacetic acid	1.25	0.95	0.30
2-Acetylphenyl N,N-dimethylcarbamate	0.93	1.27	-0.34
2-Amino-1,3-propanediol	-2.15	-2.12	-0.03
2-Amino-1,7-dihydro-6H-purine-6-thione	-0.07	-0.21	0.14
2-Amino-1-hexanol	0.6	0.27	0.33
2-Amino-1-pentanol	0.07	-0.17	0.24
2-Amino-3,3-dimethyl-1-butanol	0.34	0.03	0.31
2-Amino-4-methyl-1-pentanol	0.47	0.11	0.36
2-Amino-4-picoline	0.56	1.15	-0.59
2-Amino-4-pyrimidone	-0.99	-1.25	0.26

2-Amino-5-methylpyridine	1.02	1.15	-0.13
2-Amino-5-phenylvaleric acid	-0.36	-0.3	-0.06
2-Aminoacridine	2.62	2.77	-0.15
2-aminodiphenyl ether	2.46	2.95	-0.49
2-Aminoisobutanol	-0.59	-0.65	0.06
2-Aminopentane	1.23	1.16	0.07
2-Aminophenol	0.57	0.92	-0.35
2-Aminopyridine	0.58	0.81	-0.23
2-Aminopyrimidine	-0.22	-0.34	0.12
2-Aminoquinazolin-4-one	0.6	0.93	-0.33
2-Aminoquinoline	1.87	2.21	-0.34
2-Anthracenylisothiocyanate	5.7	5.18	0.52
2-Azacyclooctanethione	1	1.22	-0.22
2-Azacyclopentathione	-0.05	0.32	-0.37
2-Benzimidazolethiol	1.66	1.7	-0.04
2-Bromo-3-methylbutyric acid	1.48	1.68	-0.20
2-Bromoaniline	2.29	1.97	0.32
2-Bromoanisole	2.86	2.81	0.05
2-Bromobutanoic acid	1.42	1.4	0.02
2-Bromobutyric acid methyl ester	1.49	1.73	-0.24
2-Bromoethanol	0.23	0.08	0.15
2-Bromohexanoic acid	2.14	2.28	-0.14
2-Bromoisobutyric acid	0.86	1.01	-0.15
2-Bromonitrobenzene	2.51	2.75	-0.24
2-Bromooctanoic acid	3.19	3.16	0.03
2-Bromophenol	2.35	2.48	-0.13
2-Bromophenoxyacetic acid	2.1	2.12	-0.02
2-Bromophenyl N-methylcarbamate	1.77	2.1	-0.33
2-Bromophenylacetate	2.2	2.83	-0.63
2-Bromopropane	2.14	2.08	0.06
2-Bromopropanoic acid	0.92	0.96	-0.04
2-Bromopropionitrile	0.89	1.11	-0.22
2-Bromothiophenol	2.44	2.85	-0.41
2-Bromotoluene	2.92	3.22	-0.30
2-Bromovaleric acid	1.61	1.84	-0.23
2-Butanol	0.61	0.85	-0.24
2-Butanone	0.69	0.85	-0.16
2-Buten-1-ol	0.34	0.42	-0.08
2-Butylamine	0.74	0.72	0.02
2-Butylthiophenyl N-methylcarbamate	2.98	3.08	-0.10
2-Butyn-1,4-diol	-0.72	-0.73	0.01
2-Butyn-1-ol	0.37	0.34	0.03

2-Butyne	1.46	1.75	-0.29
2-Butynyl acetate	0.81	1.31	-0.50
2-Chloro-1,4-naphthoquinone	2.15	1.7	0.45
2-Chloro-1-ethylbenzene	2.95	3.54	-0.59
2-Chloro-2-methylbutane	2.52	2.78	-0.26
2-Chloro-4-phenylenediamine	0.85	0.94	-0.09
2-Chloro-5-nitro-beta-nitrostyrene	2.23	2.61	-0.38
2-Chloro-6-(trichloromethyl)pyridine	3.41	3.24	0.17
2-Chloro-6-nitrotoluene	3.09	2.97	0.12
2-Chloroaniline	1.88	1.85	0.03
2-Chloroanisole	2.5	2.69	-0.19
2-Chlorobenzenesulfonamide	0.74	0.99	-0.25
2-Chlorobenzoic acid	2.05	1.98	0.07
2-Chloro-beta-nitrostyrene	2.44	2.74	-0.30
2-Chlorobiphenyl	4.53	4.4	0.13
2-Chlorodibenzofuran	4.37	4.53	-0.16
2-Chlorodibenzo-p-dioxin	5.45	4.52	0.93
2-Chlorodiphenyl ether	4.45	4.39	0.06
2-Chloroethanol	-0.06	0	-0.06
2-Chloroisoniazid	0.11	-0.43	0.54
2-Chloronaphthalene	4.14	3.76	0.38
2-Chloronitrobenzene	2.52	2.63	-0.11
2-Chlorophenol	2.15	2.36	-0.21
2-Chlorophenoxyacetic acid	2.02	2	0.02
2-Chlorophenylacetate	2.18	2.71	-0.53
2-Chloropropane	1.9	1.96	-0.06
2-Chloropropionitrile	0.75	0.99	-0.24
2-Chloropyridine	1.28	1.53	-0.25
2-Chloroquinoline	2.71	2.93	-0.22
2-Chloroquinoxaline	2.23	1.98	0.25
2-Chlorosyringaldehyde	1.81	1.56	0.25
2-Chlorothiophenol	2.27	2.73	-0.46
2-Chlorotoluene	3.52	3.1	0.42
2-Cyano-6-methylpyridine	0.84	0.67	0.17
2-Cyanophenyl N-methylcarbamate	0.86	0.82	0.04
2-Cyanophenylacetate	1.33	1.55	-0.22
2-Decanone	3.73	3.49	0.24
2-Decyn-1-ol	3.54	2.98	0.56
2-Diethylaminoethanol	0.48	0.44	0.04
2-Dodecanone	4.55	4.37	0.18
2-Ethoxyethanol	-0.54	-0.2	-0.34
2-Ethoxyethylacetate	0.65	0.77	-0.12

2-Ethoxyphenol	1.68	2.19	-0.51
2-Ethoxyphenyl N-methylcarbamate	1.24	1.81	-0.57
2-Ethylaniline	1.74	2.1	-0.36
2-Ethylbutanoic acid	1.68	1.75	-0.07
2-Ethylbutyl acetate	2.7	2.51	0.19
2-Ethylhexanal	2.73	2.75	-0.02
2-Ethylhexanoic acid	2.64	2.63	0.01
2-Ethylhexylamine	2.82	2.33	0.49
2-Ethyl-naphthalene	4.38	4.25	0.13
2-Ethylphenoxyacetic acid	2.65	2.25	0.40
2-Ethylphenyl N-methylcarbamate	1.93	2.23	-0.30
2-Ethylphenylacetate	2.42	2.96	-0.54
2-Ethylpyridine	1.69	1.7	-0.01
2-Ethyltoluene	3.53	3.53	0.00
2-Fluoroaniline	1.38	1.34	0.04
2-Fluoroethanol	-0.92	-0.62	-0.30
2-Fluoroisoniazid	-0.11	-0.82	0.71
2-Fluorophenol	1.71	1.85	-0.14
2-Fluorophenoxyacetic acid	1.26	1.49	-0.23
2-Fluorophenyl N-methylcarbamate	1.25	1.47	-0.22
2-Fluorophenylacetate	1.76	2.2	-0.44
2-Fluorophenylacetic acid	1.5	1.91	-0.41
2-Fluoropyridine	0.84	1.14	-0.30
2-Fluorothiophenol	1.9	2.22	-0.32
2-Heptanol	2.31	2.17	0.14
2-Heptanone	1.98	2.17	-0.19
2-Heptanone oxime	2.24	1.9	0.34
2-Heptyn-1-ol	1.95	1.66	0.29
2-Hexenoic acid	1.94	1.51	0.43
2-Hexyn-1-ol	1.42	1.22	0.20
2-Hydroxyacetanilide	0.72	1.08	-0.36
2-Hydroxyacetophenone	1.92	1.82	0.10
2-Hydroxybenzaldehyde	1.7	1.68	0.02
2-Hydroxybenzamide	0.89	0.67	0.22
2-Hydroxybenzonitrile	1.61	1.2	0.41
2-Hydroxybenzophenone	3.52	3.12	0.40
2-Hydroxybenzylalcohol	0.73	1.35	-0.62
2-Hydroxybiphenyl	3.09	3.47	-0.38
2-Hydroxyphenoxyacetic acid	0.85	1.07	-0.22
2-Iodoaniline	2.32	2.33	-0.01
2-Iodobenzoic acid	2.4	2.46	-0.06
2-Iodophenol	2.65	2.84	-0.19

2-Iodophenoxyacetic acid	2.44	2.48	-0.04
2-Iodophenyl N-methylcarbamate	1.96	2.46	-0.50
2-Iodophenylacetate	2.55	3.19	-0.64
2-Isopropoxyphenol	2.09	2.66	-0.57
2-Isopropyl-5-methylphenol	3.3	3.23	0.07
2-Isopropylphenoxyacetic acid	2.84	2.53	0.31
2-Isopropylphenylacetate	2.78	3.24	-0.46
2-Isopropyltoluene	4.1	3.83	0.27
2-Methoxyacetanilide	0.98	1.41	-0.43
2-Methoxyaniline	0.95	1.25	-0.30
2-Methoxybenzamide	0.87	0.49	0.38
2-Methoxybenzylalcohol	1.13	1.68	-0.55
2-Methoxyethylamine	-0.67	-0.72	0.05
2-Methoxyisoniazid	-0.1	-0.01	-0.09
2-Methoxynitrobenzene	1.73	2.03	-0.30
2-Methoxyphenol	1.32	1.76	-0.44
2-Methoxyphenoxyacetic acid	0.98	1.4	-0.42
2-Methoxyphenyl N-methylcarbamate	0.81	1.38	-0.57
2-Methoxyquinoxaline	2.31	2.4	-0.09
2-Methyl valeraldehyde	1.67	1.87	-0.20
2-Methyl-1-propanol	0.76	0.66	0.10
2-Methyl-2-butanamine	1.1	1.12	-0.02
2-Methyl-2-butanol	0.89	1.06	-0.17
2-Methyl-2-propanol	0.37	0.62	-0.25
2-Methyl-2-propenol	0.21	0.57	-0.36
2-Methyl-4-hydroxyacetanilide	0.66	1.42	-0.76
2-Methyl-5-octyn-4-ol	2.66	2.41	0.25
2-Methyl-8-quinolinol	2.33	2.22	0.11
2-Methylaminoethanol	-0.94	-1.07	0.13
2-Methylanthracene	5	4.87	0.13
2-Methylbenzaldehyde	2.26	1.91	0.35
2-Methylbenzalmalonodinitrile	2.1	1.86	0.24
2-Methylbenzenesulfonamide	0.84	0.8	0.04
2-Methylbenzoic acid	2.46	1.79	0.67
2-Methylbenzylalcohol	1.58	1.58	0.00
2-Methyl-beta-nitrostyrene	2.63	2.55	0.08
2-Methylbutylamine	1.32	1.01	0.31
2-Methylbutyraldehyde	1.14	1.43	-0.29
2-Methylfuran	1.85	1.93	-0.08
2-Methylimidazole	0.49	-0.11	0.60
2-Methylimidazoline	0.52	0.15	0.37
2-Methylindole	2.6	3.24	-0.64

2-Methylisoniazid	-0.37	-0.7	0.33
2-Methyl-N,N'-dinitrosopiperazine	-0.28	-0.5	0.22
2-Methylnaphthalene	3.86	3.79	0.07
2-Methyl-N-nitrosopiperidine	0.71	1.23	-0.52
2-Methylphenanthrene	5.24	4.87	0.37
2-Methylphenoxyacetic acid	1.98	1.81	0.17
2-Methylphenoxyacetic acid methylester	2.08	2.14	-0.06
2-Methylpropanal	0.61	0.99	-0.38
2-Methylpropane	2.76	2.35	0.41
2-Methylpropanoic acid	0.6	0.87	-0.27
2-Methylpropenoic acid	0.93	0.78	0.15
2-Methylpropylamine	0.73	0.57	0.16
2-Methylpyrazine	0.23	-0.09	0.32
2-Methylquinoline	2.59	2.66	-0.07
2-Methylquinoxaline	1.61	1.71	-0.10
2-Naphthol	2.7	2.83	-0.13
2-Naphthoxyacetic acid	2.53	2.47	0.06
2-Naphthylamine	2.28	2.32	-0.04
2-Naphthylisothiocyanate	4.34	4.18	0.16
2-Nitroaniline	1.85	1.7	0.15
2-Nitrobenzaldehyde	1.74	1.44	0.30
2-Nitrobenzenesulfonamide	0.34	0.84	-0.50
2-Nitrobenzoic acid	1.47	1.83	-0.36
2-Nitroethanol	-0.42	-0.92	0.50
2-Nitroethylbenzene	2.08	2.15	-0.07
2-Nitro-m-xylene	2.95	2.78	0.17
2-Nitrophenol	1.77	2.21	-0.44
2-Nitrophenoxyacetic acid	1.22	1.34	-0.12
2-Nitrophenyl N-methylcarbamate	1.02	1.32	-0.30
2-Nitrophenylacetate	1.55	2.05	-0.50
2-Nitropropane	0.93	0.81	0.12
2-Nitroresorcinol	1.36	2.32	-0.96
2-Nitrotoluene	2.3	2.44	-0.14
2-Nonanone	3.14	3.05	0.09
2-Nonyn-1-ol	3.01	2.54	0.47
2-Nonynoic acid	2.65	2.75	-0.10
2-n-Propylphenol	2.93	3.05	-0.12
2-Octanol	2.9	2.61	0.29
2-Octanone	2.37	2.61	-0.24
2-Octen-1-ol	2.45	2.18	0.27
2-Octyn-1-ol	2.48	2.1	0.38
2-Octynoic acid	2.12	2.31	-0.19

2-Penten-4-yn-1-ol	-0.01	0.08	-0.09
2-Pentyn-1-ol	0.89	0.78	0.11
2-Phenethylisothiocyanate	3.74	3.97	-0.23
2-Phenoxyanisole	2.92	3.79	-0.87
2-Phenoxybenzoic acid	2.84	3.59	-0.75
2-Phenoxyethanol	1.16	1.26	-0.10
2-Phenylaniline	3.34	2.96	0.38
2-Phenylethylamine	1.41	1.59	-0.18
2-Phenylimidazole	1.88	1.19	0.69
2-Phenylphenoxyacetic acid	2.83	3.11	-0.28
2-Phenylpyridine	2.63	2.56	0.07
2-Phenylquinoline	3.9	3.96	-0.06
2-Phenylthiophene	3.74	3.62	0.12
2-Picoline	1.11	1.26	-0.15
2-Propanol	0.26	0.41	-0.15
2-Propylpentanoic acid	2.75	2.63	0.12
2-Propyn-1-ol	-0.38	-0.4	0.02
2-Pyridinecarbonitrile	0.4	0.29	0.11
2-Pyridinemethanamine	-0.21	-0.16	-0.05
2-Pyridinemethanol	0.06	-0.07	0.13
2-Pyridinepropanol	0.58	0.81	-0.23
2-Pyridone	-0.58	0.21	-0.79
2-Pyrimidone	-1.62	-2.21	0.59
2-Pyrrolidone	0.46	-0.01	0.47
2-s-Butylphenol	3.27	3.33	-0.06
2-s-Butylphenoxyacetic acid	3.32	2.97	0.35
2-s-Butylphenyl N,N-dimethylcarbamate	3.31	3.29	0.02
2-s-Butylphenyl N-methylcarbamate	2.78	2.95	-0.17
2-t-Butylphenol	3.31	3.25	0.06
2-t-Butylphenoxyacetic acid	3.33	2.89	0.44
2-t-Butylphenyl N-methylcarbamate	2.65	2.87	-0.22
2-Thiocresol	3.52	2.54	0.98
2-Thiouracil	-0.28	-0.63	0.35
2-Tolunitrile	2.21	1.94	0.27
2-Tolyl N-methylcarbamate	1.46	1.79	-0.33
2-Tridecanone	5.08	4.81	0.27
2-Tridecyn-1-ol	5.13	4.3	0.83
2-Trifluoromethylbenzimidazole	2.67	2.42	0.25
2-Trifluoromethylphenol	2.8	2.76	0.04
2-Undecanone	4.09	3.93	0.16
3-(1-Methyl-2-pyrrolidinyl)pyridine	1.17	1.24	-0.07
3-(2-pyridyl)propionamide	-0.27	0.13	-0.40

3-(2-Pyridyl)propylamine	0.49	0.72	-0.23
3-(3-pyridyl)propionamide	-0.26	0.09	-0.35
3-(3-Pyridyl)propylamine	0.44	0.68	-0.24
3-(4-Pyridyl)propanol	0.58	0.77	-0.19
3-(4-pyridyl)propionamide	-0.25	0.09	-0.34
3-(4-Pyridyl)propylamine	0.4	0.68	-0.28
3-(Dimethylamino)benzamide	0.95	0.25	0.70
3-(Dimethylamino)phenyl N-methylcarbamate	1.43	1.14	0.29
3-(Methylthio)aniline	1.45	1.79	-0.34
3-(Trifluoromethylsulfonyl)phenoxyacetic acid	2.19	1.84	0.35
3-(Trifluoromethylthio)phenoxyacetic acid	2.86	3.32	-0.46
3,3',4,4',5,5'-Hexachlorobiphenyl	7.41	7.05	0.36
3,3',4,4',5-Pentabromodiphenyl ether	6.97	7.11	-0.14
3,3',4,4',5-Pentachlorodiphenyl ether	6.88	6.51	0.37
3,3',4,4'-Tetrabromodiphenyl ether	6.96	6.46	0.50
3,3',4,4'-Tetrachlorobiphenyl	6.63	5.99	0.64
3,3',4,4'-Tetrachlorodiphenyl ether	6.36	5.98	0.38
3,3',4-Tribromodiphenyl ether	5.58	5.81	-0.23
3,3',5,5'-Tetrachlorobiphenyl	6.48	5.99	0.49
3,3',5-Trichlorobiphenyl	5.81	5.46	0.35
3,3'-Dichlorobenzidine	3.51	3.11	0.40
3,3'-Dichlorobiphenyl	5.3	4.93	0.37
3,3-Dimethyl-2-butanol	1.48	1.49	-0.01
3,3-Dimethylbutyraldehyde	1.63	1.79	-0.16
3,3-Dimethylglutaric acid	0.16	0.84	-0.68
3,4,4'-Tribromodiphenyl ether	5.58	5.81	-0.23
3,4,4'-Trichlorobiphenyl	5.78	5.46	0.32
3,4,5,6-Tetrachloroguaiacol	4.42	3.88	0.54
3,4,5-Trichlorocatechol	3.75	3.02	0.73
3,4,5-Trichloroguaiacol	3.77	3.35	0.42
3,4,5-Trichloroveratrole	4.01	3.68	0.33
3,4,5-Trimethylphenol	2.87	2.85	0.02
3,4-Diaminobenzoic acid	-0.7	-0.37	-0.33
3,4-Diaminofurazan	0.02	-0.26	0.28
3,4'-Dibromodiphenyl ether	5.03	5.16	-0.13
3,4-Dibromodiphenyl ether	5.03	5.16	-0.13
3,4-Dibromohexane	3.85	3.77	0.08
3,4-Dichloroaniline	2.69	2.38	0.31
3,4-Dichlorobenzenesulfonamide	1.44	1.52	-0.08
3,4'-Dichlorobiphenyl	5.15	4.93	0.22
3,4-Dichlorobiphenyl	5.29	4.93	0.36
3,4-Dichloronitrobenzene	3.12	3.16	-0.04

3,4-Dichlorophenol	3.33	2.89	0.44
3,4-Dichlorophenoxyacetic acid	2.81	2.53	0.28
3,4-Dichlorophenyl N-methylcarbamate	2.8	2.51	0.29
3,4-Dichlorotoluene	3.95	3.63	0.32
3,4-Dihydro-2H-1-benzopyran-2-one	1.67	2.72	-1.05
3,4-Dimethoxyamphetamine	1	1.88	-0.88
3,4-Dimethylphenyl N-methylcarbamate	2.09	2.13	-0.04
3,4-Dimethylthiophenol	3.62	2.88	0.74
3,4-Diphenyl-1,2,5-oxadiazole	3.84	4	-0.16
3,4-Xylenol	2.23	2.51	-0.28
3,4-Xylidine	1.86	2	-0.14
3,5-Dibromo-4-hydroxybenzonitrile	2.6	2.5	0.10
3,5-Dichloroaniline	2.9	2.38	0.52
3,5-Dichlorobiphenyl	5.41	4.93	0.48
3,5-Dichloronitrobenzene	3.09	3.16	-0.07
3,5-Dichlorophenol	3.61	2.89	0.72
3,5-Dichlorophenyl N-methylcarbamate	3.03	2.51	0.52
3,5-Dichloropyridine	2.56	1.94	0.62
3,5-Dichlorothiophenol	2.43	3.26	-0.83
3,5-Diethyl-4-hydroxyacetanilide	2.36	2.64	-0.28
3,5-Diiodosalicylic acid	4.56	3.58	0.98
3,5-Dimethyl-4-hydroxyacetanilide	1.6	1.76	-0.16
3,5-Dimethyl-N-nitrosopiperidine	1.53	1.36	0.17
3,5-Dinitro-4-methylbenzamide	0.68	0.64	0.04
3,5-Dinitrophenol	2.32	1.57	0.75
3,5-Dipropyl-4-hydroxyacetanilide	3.16	3.52	-0.36
3,5-Dithiaheptane	2.64	2.53	0.11
3,5-Heptanedione	0.6	0.87	-0.27
3,5-Xylenol	2.35	2.51	-0.16
3,6-Acridinediamine	1.4	1.86	-0.46
3,6-Dichlorodibenzofuran	5.44	5.06	0.38
3,6-Dichloropicolinic acid	1.07	1.32	-0.25
3,beta-Dinitrostyrene	1.82	2.08	-0.26
3-Acetamido-4-chlorophenoxyacetic acid	0.67	1.25	-0.58
3-Acetamidophenol	0.73	1.08	-0.35
3-Acetamidophenoxyacetic acid	0.48	0.72	-0.24
3-Acetaminpyridine	0.41	0.13	0.28
3-Acetylaminoquinoline	1.92	1.53	0.39
3-Acetylphenoxyacetic acid	0.98	0.95	0.03
3-Acetylphenyl N,N-dimethylcarbamate	1.18	1.27	-0.09
3-Acetylphenyl N-methylcarbamate	0.9	0.93	-0.03
3-Acetylpyridine	0.43	0.36	0.07

3-Allyloxy-4-aminobenzoic acid	0.42	1.12	-0.70
3-Amino-1,2-propanediol,	-2.12	-1.57	-0.55
3-Amino-2,2-dimethyl-1-propanol	-0.79	-0.4	-0.39
3-Amino-4-chlorophenoxyacetic acid	1.16	1.09	0.07
3-Amino-4-phenyl-1,2,5-oxadiazole	1.81	1.87	-0.06
3-Aminoacridine	2.19	2.77	-0.58
3-Aminobenzamide	0.33	-0.35	0.68
3-Aminobenzenesulfonamide	-1.2	-0.45	-0.75
3-Aminobenzylalcohol	-0.55	0.33	-0.88
3-Aminopentane	1.23	1.16	0.07
3-Aminophenol	0.17	0.92	-0.75
3-Aminopyridine	0.11	-0.03	0.14
3-Aminoquinoline	1.63	1.37	0.26
3-Benzamidophenoxyacetic acid	1.99	2.02	-0.03
3-Bromo-1-propanol	0.15	0.52	-0.37
3-Bromo-2,2-dimethyl-1-propanol	0.95	1.16	-0.21
3-Bromo-4-chlorophenoxyacetic acid	2.75	2.65	0.10
3-Bromoaniline	2.1	1.97	0.13
3-Bromobenzamide	1.65	1.21	0.44
3-Bromobenzoic acid	2.87	2.1	0.77
3-Bromochlorobenzene	3.7	3.41	0.29
3-Bromonitrobenzene	2.64	2.75	-0.11
3-Bromophenol	2.63	2.48	0.15
3-Bromophenoxyacetic acid	2.22	2.12	0.10
3-Bromophenyl N-methylcarbamate	2.25	2.1	0.15
3-Bromophenylacetic acid	2.37	2.54	-0.17
3-Bromopropionic acid	0.5	0.73	-0.23
3-Bromopyridine	1.6	1.53	0.07
3-Bromoquinoline	2.91	2.93	-0.02
3-Bromothiophenol	2.48	2.85	-0.37
3-Bromotoluene	3.43	3.22	0.21
3-Buten-2-ol	0.12	0.63	-0.51
3-Butenoic acid	0.34	0.81	-0.47
3-Butoxyphenyl N-methylcarbamate	2.96	2.69	0.27
3-Butylphenoxyacetic acid	3.18	3.13	0.05
3-Butyn-2-ol	0.14	0.07	0.07
3-Carbamidomethylpyridine	-0.71	-0.35	-0.36
3-Carboxyphenol	1.5	1.05	0.45
3-Carboxyphenoxyacetic acid	1.11	0.54	0.57
3-Carboxyphenylacetic acid	1.14	0.96	0.18
3-Chloro-1-propanol	0.5	0.44	0.06
3-Chloro-2,2-dimethyl-1-propanol	0.81	1.08	-0.27

3-Chloro-2,4-pentanedione	0.05	0.24	-0.19
3-Chloro-2-butanone	0.43	1.1	-0.67
3-Chloro-5-fluorophenoxyacetic acid	2.2	2.02	0.18
3-Chloroaniline	1.88	1.85	0.03
3-Chloroanisole	2.6	2.69	-0.09
3-Chlorobenzamide	1.51	1.09	0.42
3-Chlorobenzenesulfonamide	1.29	0.99	0.30
3-Chlorobenzoic acid	2.68	1.98	0.70
3-Chlorobenzylalcohol	1.94	1.77	0.17
3-Chloro-beta-nitrostyrene	2.57	2.74	-0.17
3-Chlorobiphenyl	4.58	4.4	0.18
3-Chlorodibenzofuran	4.35	4.53	-0.18
3-Chloronitrobenzene	2.46	2.63	-0.17
3-Chlorophenol	2.5	2.36	0.14
3-Chlorophenoxyacetic acid	2.03	2	0.03
3-Chlorophenyl N-methylcarbamate	2.03	1.98	0.05
3-Chlorophenylacetate	2.32	2.71	-0.39
3-Chlorophenylacetic acid	2.09	2.42	-0.33
3-Chloropropionic acid	0.41	0.65	-0.24
3-Chloropropionitrile	0.18	0.8	-0.62
3-Chloropyridine	1.33	1.41	-0.08
3-Chlorothiophenol	2.47	2.73	-0.26
3-Chlorotoluene	3.28	3.1	0.18
3-Cyanobenzamide	0.52	-0.07	0.59
3-Cyanobenzoic acid	1.48	0.82	0.66
3-Cyanophenol	1.7	1.2	0.50
3-Cyanophenoxyacetic acid	0.95	0.84	0.11
3-Cyanophenyl N-methylcarbamate	0.97	0.82	0.15
3-Cyanophenylacetic acid	1.18	1.26	-0.08
3-Decanone	3.49	3.49	0.00
3-Decyn-1-ol	2.99	2.98	0.01
3-Dimethylaminophenol	1.57	1.52	0.05
3-Ethoxyphenol	1.98	2.19	-0.21
3-Ethoxyphenyl N-methylcarbamate	1.75	1.81	-0.06
3-Ethoxypropylamine	-0.49	0.15	-0.64
3-Ethyl-1-hydroxyurea	-0.76	-0.91	0.15
3-Ethyl-4-hydroxyacetanilide	1.79	1.86	-0.07
3-Ethylphenol	2.5	2.61	-0.11
3-Ethylphenoxyacetic acid	2.25	2.25	0.00
3-Ethylphenyl N-methylcarbamate	2.2	2.23	-0.03
3-Ethyltoluene	3.88	3.53	0.35
3-Fluoro-5-iodophenoxyacetic acid	2.42	2.5	-0.08

3-Fluoroaniline	1.3	1.34	-0.04
3-Fluorobenzalmalonodiamide	0.1	-0.54	0.64
3-Fluorobenzamide	0.91	0.58	0.33
3-Fluorobenzoic acid	2.15	1.47	0.68
3-Fluorobenzyl chloride	2.77	2.65	0.12
3-Fluorophenol	1.93	1.85	0.08
3-Fluorophenoxyacetic acid	1.48	1.49	-0.01
3-Fluorophenyl N-methylcarbamate	1.48	1.47	0.01
3-Fluorophenylacetate	1.74	2.2	-0.46
3-Fluorophenylacetic acid	1.65	1.91	-0.26
3-Fluorothiophenol	2.12	2.22	-0.10
3-Heptanol	2.24	2.17	0.07
3-Heptanone	1.73	2.17	-0.44
3-Heptyn-1-ol	1.4	1.66	-0.26
3-Hexyn-1-ol	0.87	1.22	-0.35
3-Hexyn-2-ol	1.2	1.25	-0.05
3-Hexyne-2,5-diol	-0.1	0.21	-0.31
3-Hydroxyacetophenone	1.39	1.31	0.08
3-Hydroxybenzamide	0.39	0.16	0.23
3-Hydroxybenzylalcohol	0.49	0.84	-0.35
3-Hydroxy-beta-nitrostyrene	2.07	1.81	0.26
3-Hydroxybiphenyl	3.23	3.47	-0.24
3-Hydroxy-N-Nitrosopiperidine	-0.47	-0.5	0.03
3-Hydroxyphenoxyacetic acid	0.76	1.07	-0.31
3-Hydroxyphenylacetate	1.23	1.78	-0.55
3-Hydroxyphenylacetic acid	0.85	1.49	-0.64
3-Hydroxypicolinic acid	-1.27	-1.14	-0.13
3-Iodoaniline	2.86	2.33	0.53
3-Iodobenzoic acid	3.13	2.46	0.67
3-Iodonitrobenzene	2.94	3.11	-0.17
3-Iodophenol	2.93	2.84	0.09
3-Iodophenoxyacetic acid	2.62	2.48	0.14
3-Iodophenyl N-methylcarbamate	2.52	2.46	0.06
3-Isopropoxyphenyl N-methylcarbamate	1.96	2.28	-0.32
3-Isopropyl-4-hydroxyacetanilide	2.2	2.14	0.06
3-Isopropylphenoxyacetic acid	2.59	2.53	0.06
3-Methoxy-4-hydroxybenzaldehyde	1.21	1.1	0.11
3-Methoxybenzalmalonodiamide	0.01	-0.12	0.13
3-Methoxybenzamide	0.94	0.49	0.45
3-Methoxy-beta-nitrostyrene	2.37	2.14	0.23
3-Methoxycarbonylphenyl N-methylcarbamate	1.42	1	0.42
3-Methoxyformanilide	1.25	1.2	0.05

3-Methoxyphenol	1.58	1.76	-0.18
3-Methoxyphenoxyacetic acid	1.38	1.4	-0.02
3-Methoxyphenyl N,N-dimethylcarbamate	1.6	1.72	-0.12
3-Methoxyphenyl N-methylcarbamate	1.3	1.38	-0.08
3-Methoxyphenylacetic acid	1.5	1.82	-0.32
3-Methoxysalicylaldehyde	1.37	1.61	-0.24
3-Methoxythiophenol	2.93	2.13	0.80
3-Methoxytoluene	2.66	2.5	0.16
3-Methyl-2-butanol	1.28	1.13	0.15
3-Methyl-2-butanone	0.84	1.13	-0.29
3-Methyl-4-hydroxyacetanilide	1.28	1.42	-0.14
3-Methyl-4-methylthiophenyl N-methylcarbamate	2.47	2.26	0.21
3-Methyl-4-nitroquinoline-1-oxide	1.06	1.1	-0.04
3-Methyl-4-phenyl-1,2,5-oxadiazole	2.59	2.7	-0.11
3-Methylamino-1,2-propanediol	-1.82	-1.67	-0.15
3-Methylbenzalmalonodiamide	0.4	0.29	0.11
3-Methylbenzenesulfonamide	0.85	0.8	0.05
3-Methylbenzoic acid	2.37	1.79	0.58
3-Methylbenzylalcohol	1.6	1.58	0.02
3-Methylbutanoic acid	1.16	1.31	-0.15
3-Methylcholanthrene	6.42	6.87	-0.45
3-Methyl-N-nitrosopiperidine	0.99	1.08	-0.09
3-Methylpentane	3.6	3.41	0.19
3-Methylphenanthrene	5.15	4.87	0.28
3-Methylphenoxyacetic acid	1.78	1.81	-0.03
3-Methylpyridine	1.2	1.22	-0.02
3-Methylquinazolin-4-one	0.69	0.39	0.30
3-Methylstyrene	3.35	3.31	0.04
3-Methylthiophenoxyacetic acid	1.9	1.94	-0.04
3-Methylvaleric acid	1.75	1.75	0.00
3-Nitroacetophenone	1.42	1.58	-0.16
3-Nitroaniline	1.37	1.19	0.18
3-Nitroanisole	2.16	2.03	0.13
3-Nitrobenzaldehyde	1.47	1.44	0.03
3-Nitrobenzamide	0.77	0.43	0.34
3-Nitrobenzenesulfonamide	0.55	0.33	0.22
3-Nitrobenzoic acid	1.89	1.32	0.57
3-Nitrobenzonitrile	1.17	1.47	-0.30
3-Nitrobenzylalcohol	1.21	1.11	0.10
3-Nitrophenol	2	1.7	0.30
3-Nitrophenoxyacetic acid	1.37	1.34	0.03
3-Nitrophenyl N-methylcarbamate	1.39	1.32	0.07

3-Nitrophenylacetate	1.82	2.05	-0.23
3-Nitrophenylacetic acid	1.45	1.76	-0.31
3-Nitropyridine	0.6	0.75	-0.15
3-Nitroquinoline	1.97	2.15	-0.18
3-Nitroquinoline-1-oxide	0.56	0.76	-0.20
3-Nitrotoluene	2.45	2.44	0.01
3-Nonyn-1-ol	2.46	2.54	-0.08
3-Octyn-1-ol	1.93	2.1	-0.17
3-p-Anisoyl-3-bromoacrylic acid	1.74	1.7	0.04
3-Pentanol	1.21	1.29	-0.08
3-Penten-2-ol	0.65	0.89	-0.24
3-Pentyn-1-ol	0.34	0.78	-0.44
3-Phenyl-1-iodopropane	3.9	4.26	-0.36
3-Phenylphenoxyacetic acid	3.18	3.11	0.07
3-Phenylpropanoic acid	1.84	2.33	-0.49
3-Phenylpropene	3.23	3.41	-0.18
3-Phenylpropionamide	1.03	1.44	-0.41
3-Phenylpropylamine	1.83	2.03	-0.20
3-Phenylpropyldimethylamine	2.73	2.85	-0.12
3-Phenylpropylfluoride	2.95	2.89	0.06
3-Propionylphenyl N-methylcarbamate	1.49	1.37	0.12
3-Propylphenoxyacetic acid	2.71	2.69	0.02
3-Pyridinecarbonitrile	0.36	0.25	0.11
3-Pyridinemethanamine	-0.32	-0.2	-0.12
3-Pyridinemethanol	-0.02	-0.11	0.09
3-Pyridinepropanol	0.6	0.77	-0.17
3-t-Butyl-4-hydroxyacetanilide	2.85	2.5	0.35
3-t-Butylphenyl N-methylcarbamate	2.93	2.87	0.06
3-Tetradecyn-1-ol	5.11	4.74	0.37
3-Thiocresol	3.13	2.54	0.59
3-Thiopropionic acid	0.43	0.64	-0.21
3-Trifluoromethylbenzoic acid	2.95	2.38	0.57
3-Trifluoromethylphenol	2.95	2.76	0.19
3-Trifluoromethylphenoxyacetic acid	2.36	2.4	-0.04
3-Trifluoromethylphenylacetic acid	2.62	2.82	-0.20
3-Ureidophenoxyacetic acid	0.26	0.16	0.10
4-(2,4-Dichlorophenoxy)butyric acid	3.53	3.41	0.12
4-(2-Pyridyl)butanol	0.86	1.25	-0.39
4-(2-Pyridyl)butylamine	0.86	1.16	-0.30
4-(2-Pyridyl)pentamide	-0.01	0.85	-0.86
4(3H)-Pyridmidone	-1.38	-1.05	-0.33
4-(3-Pyridyl)butanamide	-0.08	0.53	-0.61

4-(3-Pyridyl)butanol	0.92	1.21	-0.29
4-(3-Pyridyl)butylamine	0.88	1.12	-0.24
4-(4-Pyridyl)butanamide	-0.09	0.53	-0.62
4-(4-Pyridyl)butanol	0.9	1.21	-0.31
4-(4-Pyridyl)butylamine	0.86	1.12	-0.26
4-(Acetylamino)benzamide	0.01	-0.19	0.20
4-(Acetylamino)benzoic acid	1.31	0.7	0.61
4-(Dimethylamino)benzamide	1.14	0.25	0.89
4-(Methylthio)benzoic acid	2.74	1.92	0.82
4-(Methylthio)phenol	1.78	2.3	-0.52
4-(Methylthio)phenyl N-methylcarbamate	1.92	1.92	0.00
4,4'-Diaminodiphenyl sulfone	0.97	1.07	-0.10
4,4'-Dibromobiphenyl	5.72	5.17	0.55
4,4'-Dibromodiphenyl ether	5.03	5.16	-0.13
4,4'-Dichlorobiphenyl	5.58	4.93	0.65
4,4'-Diisothiocyanatobiphenyl	5.5	5.77	-0.27
4,4'-Dimethylbiphenyl	5.09	4.83	0.26
4,5,6-Trichloro-2-trifluoromethylbenzimidazole	4.08	4.01	0.07
4,5,6-Trichloroguaiacol	3.72	3.35	0.37
4,5,7-Trichloro-2-trifluoromethylbenzimidazole	3.78	4.01	-0.23
4,5-Dibromo-1,2,3-triazole	2.24	3.01	-0.77
4,5-Dichloroguaiacol	3.26	2.82	0.44
4,5-Dichloroveratrole	3.11	3.15	-0.04
4,5-Diethyldibenzothiophene	5.98	6.07	-0.09
4,5-Dimethyl-8-quinolinol	2.71	2.56	0.15
4,5-Dimethyldibenzothiophene	5.97	5.19	0.78
4,5-Dinitroquinoline-1-oxide	0.95	0.63	0.32
4,6-Dichloro-2-trifluoromethylbenzimidazole	3.49	3.48	0.01
4,6-Dimethylpyrimidine	0.62	0.61	0.01
4,6-Dinitro-o-cresol	2.12	2.42	-0.30
4,6-Dinitroquinoline-1-oxide	0.9	0.63	0.27
4,7-Dichloro-2-trifluoromethylbenzimidazole	2.87	3.48	-0.61
4,7-Phenanthroline	2.05	2.33	-0.28
4,beta-Dinitrostyrene	1.89	2.08	-0.19
4-Acetaminpyridine	0.59	0.13	0.46
4-Acetyl-7-chloroquinoline	2.62	2.29	0.33
4-Acetylanisole	1.82	1.64	0.18
4-Acetylformanilide	0.94	0.75	0.19
4-Acetylphenol	1.35	1.31	0.04
4-Acetylphenoxyacetic acid	0.87	0.95	-0.08
4-Acetylphenyl N-methylcarbamate	1.01	0.93	0.08
4-Acetylpyridine	0.54	0.36	0.18

4-Allyl-2-methoxyphenol	2.27	2.76	-0.49
4-Amino-1-butanol	-1.06	-0.6	-0.46
4-Amino-2-bromobenzoic acid	0.66	1.19	-0.53
4-Amino-2-butoxybenzoic acid	1.24	2.29	-1.05
4-Amino-2-chlorobenzoic acid	0.5	1.07	-0.57
4-Amino-2-ethoxybenzoic acid	0.16	0.9	-0.74
4-Amino-2-fluorobenzoic acid	0.46	0.56	-0.10
4-Amino-2-iodobenzoic acid	0.82	1.55	-0.73
4-Amino-2-isopentoxybenzoic acid	1.47	2.57	-1.10
4-Amino-2-methoxybenzoic acid	-0.38	0.47	-0.85
4-Amino-2-methylbenzoic acid	0.31	0.88	-0.57
4-Amino-2-nitrobenzoic acid	0.38	0.41	-0.03
4-Amino-2-nitrophenol	0.96	1.3	-0.34
4-Amino-2-pentoxybenzoic acid	1.55	2.73	-1.18
4-Amino-2-propoxybenzoic acid	0.7	1.85	-1.15
4-Amino-3,5,6-trichloro-2-pyridinecarboxylic acid	0.3	0.94	-0.64
4-Amino-3-bromobenzoic acid	1.4	1.19	0.21
4-Amino-3-chlorobenzoic acid	1.52	1.07	0.45
4-Amino-3-fluorobenzoic acid	0.58	0.56	0.02
4-Amino-3-hydroxybenzoic acid	-0.32	0.14	-0.46
4-Amino-3-iodobenzoic acid	1.53	1.55	-0.02
4-Amino-3-methylbenzoic acid	0.54	0.88	-0.34
4-Amino-3-methylthio-6-propyl-1,2,4-triazine-5-one	1.01	1.28	-0.27
4-Amino-3-morpholino-6-isopropyl-1,2,4-triazine-5-one	0.49	0.16	0.33
4-Amino-6-isopentyl-3-methylthio-1,2,4-triazin-5-one	1.85	2	-0.15
4-Amino-6-isopropyl-3-isopropylthio-1,2,4-triazin-5-one	2.06	1.79	0.27
4-Amino-6-isopropyl-3-propylthio-1,2,4-triazin-5-one	2.12	1.84	0.28
4-Amino-6-methyl-3-(methylthio)-1,2,4-triazin-5-one	-0.16	0.4	-0.56
4-Amino-6-phenyl-3-(methylthio)-1,2,4-triazin-5-one	1.66	1.7	-0.04
4-Aminoacetanilide	0.08	0.57	-0.49
4-Aminoacetophenone	0.41	0.8	-0.39
4-Aminoacridine	3.26	2.77	0.49
4-Aminobenzamide	0.02	-0.35	0.37
4-Aminobenzenesulfonamide	-0.78	-0.45	-0.33
4-aminodiphenyl ether	2.36	2.95	-0.59
4-Aminophenol	0.04	0.92	-0.88
4-Aminophenylacetate	0.45	1.27	-0.82
4-Aminopyridine	0.28	-0.03	0.31
4-Aminopyrimidine	-0.25	-0.22	-0.03
4-Aminoquinoline	1.63	1.37	0.26
4-Aminoquinoline-1-oxide	0.05	-0.02	0.07
4-Aminosalicylic acid	0.87	0.65	0.22

4-Aminosalicylic acid 2-bromophenylester	3.74	3.33	0.41
4-Aminosalicylic acid 2-chlorophenylester	3.72	3.21	0.51
4-Aminosalicylic acid 2-fluorophenylester	3.29	2.7	0.59
4-Aminosalicylic acid 2-methoxyphenylester	2.88	2.61	0.27
4-Aminosalicylic acid 2-tolylester	3.14	3.02	0.12
4-Aminosalicylic acid 3-bromophenylester	3.84	3.33	0.51
4-Aminosalicylic acid 3-chlorophenylester	3.9	3.21	0.69
4-Aminosalicylic acid 3-fluorophenylester	3.42	2.7	0.72
4-Aminosalicylic acid 3-methoxyphenylester	3.25	2.61	0.64
4-Aminosalicylic acid 3-tolylester	3.64	3.02	0.62
4-Aminosalicylic acid 4-bromophenylester	3.46	3.33	0.13
4-Aminosalicylic acid 4-chlorophenylester	3.6	3.21	0.39
4-Aminosalicylic acid 4-fluorophenylester	3.27	2.7	0.57
4-Aminosalicylic acid 4-methoxyphenylester	3.07	2.61	0.46
4-Aminosalicylic acid 4-tolylester	3.38	3.02	0.36
4-Aminothiophenol	1.88	1.29	0.59
4-Benzoylphenol	3.07	2.61	0.46
4-Benzoylpyridine	1.98	1.66	0.32
4-Benzylphenylisothiocyanate	4.4	5.26	-0.86
4-Biphenylisothiocyanate	4.66	4.82	-0.16
4-Bromo-1-butene	2.53	2.07	0.46
4-Bromo-2,6-dimethylphenyl isocyanate	3.63	3.62	0.01
4-Bromo-3,5-dimethoxyphenethylamine	2.03	2.1	-0.07
4-Bromoacetophenone	2.43	2.36	0.07
4-Bromoaniline	2.26	1.97	0.29
4-Bromobenzamide	1.76	1.21	0.55
4-Bromobenzenesulfonamide	1.36	1.11	0.25
4-Bromobenzoic acid	2.86	2.1	0.76
4-Bromobiphenyl	4.95	4.52	0.43
4-Bromobutyl acetate	1.62	1.93	-0.31
4-Bromobutyric acid	0.68	1.17	-0.49
4-Bromobutyronitrile	0.52	1.32	-0.80
4-Bromonitrobenzene	2.55	2.75	-0.20
4-Bromophenol	2.43	2.48	-0.05
4-Bromophenoxyacetic acid	2.45	2.12	0.33
4-Bromophenyl N-methylcarbamate	2.17	2.1	0.07
4-Bromophenylacetic acid	2.31	2.54	-0.23
4-Bromophenylisothiocyanate	4.03	3.83	0.20
4-Bromopyridine	1.54	1.53	0.01
4-Bromothiophenol	2.72	2.85	-0.13
4-Bromotoluene	3.42	3.22	0.20
4-Butoxybenzamide	2.48	1.8	0.68

4-Butoxyphenol	2.87	3.07	-0.20
4-Butoxyphenyl N-methylcarbamate	2.86	2.69	0.17
4-Butylaniline	3.18	2.98	0.20
4-Butylbenzenesulfonamide	2.45	2.12	0.33
4-Carbamidomethylpyridine	-0.65	-0.35	-0.30
4-Carboxyphenol	1.58	1.05	0.53
4-Carboxyphenylisothiocyanate	3.52	2.4	1.12
4-Chloro-1-butanol	0.85	0.88	-0.03
4-Chloro-2,5-dimethylphenyl N-methylcarbamate	2.95	2.66	0.29
4-Chloro-2-methylphenol	2.78	2.7	0.08
4-Chloro-2-nitrotoluene	3.05	2.97	0.08
4-Chloro-2-trifluoromethylbenzimidazole	2.93	2.95	-0.02
4-Chloro-3-cyanophenoxyacetic acid	1.56	1.37	0.19
4-Chloro-3-iodophenoxyacetic acid	3.1	3.01	0.09
4-Chloro-3-nitrophenoxyacetic acid	1.85	1.87	-0.02
4-Chloro-6-nitro-m-cresol	2.93	3.08	-0.15
4-Chloro-8-quinolinol	2.67	2.41	0.26
4-Chloroacetanilide	1.87	2.01	-0.14
4-Chloroacetophenone	2.35	2.24	0.11
4-Chloroaniline	1.83	1.85	-0.02
4-Chloroanisole	2.78	2.69	0.09
4-Chlorobenzaldehyde	2.13	2.1	0.03
4-Chlorobenzamide	1.51	1.09	0.42
4-Chlorobenzenesulfonamide	0.84	0.99	-0.15
4-Chlorobenzoic acid	2.65	1.98	0.67
4-Chlorobenzylalcohol	1.96	1.77	0.19
4-Chloro-beta-nitrostyrene	2.85	2.74	0.11
4-Chlorobiphenyl	4.61	4.4	0.21
4-Chlorobutanoic acid	0.54	1.09	-0.55
4-Chlorobutyronitrile	0.56	1.24	-0.68
4-Chlorodiphenyl ether	4.08	4.39	-0.31
4-Chloro-m-cresol	3.1	2.7	0.40
4-Chloronitrobenzene	2.39	2.63	-0.24
4-Chlorophenol	2.39	2.36	0.03
4-Chlorophenoxyacetic acid	1.99	2	-0.01
4-Chlorophenylacetic acid	2.12	2.42	-0.30
4-Chloroquinoline-1-oxide	1.08	1.42	-0.34
4-Chlorothiophenol	2.66	2.73	-0.07
4-Chlorotoluene	3.33	3.1	0.23
4-Cumylphenyl diphenyl phosphate	6.1	6.88	-0.78
4-Cyano-2-methylpyridine	0.81	0.63	0.18
4-Cyanobenzamide	0.48	-0.07	0.55

4-Cyanobenzenesulfonamide	0.23	-0.17	0.40
4-Cyanobenzoic acid	1.56	0.82	0.74
4-Cyanoformanilide	1.08	0.64	0.44
4-Cyano-N-formylstyrylamine	1.58	0.73	0.85
4-Cyanophenoxyacetic acid	0.93	0.84	0.09
4-Cyanophenyl N-methylcarbamate	0.95	0.82	0.13
4-Cyanopyrazole	0.24	0.49	-0.25
4-Cyanopyridine	0.46	0.25	0.21
4-Cyclohexylphenoxyacetic acid	3.79	3.35	0.44
4-Cyclopentylphenoxyacetic acid	3.41	3.05	0.36
4-Cyclopropyl-2-butanone	1.5	1.93	-0.43
4-Diethylaminobenzylalcohol	2.29	2.03	0.26
4-Dimethylamino-beta-nitrostyrene	2.67	1.9	0.77
4-Ethoxyacetanilide	1.58	1.84	-0.26
4-Ethoxybenzamide	1.3	0.92	0.38
4-Ethoxyphenol	1.81	2.19	-0.38
4-Ethoxyphenyl N-methylcarbamate	1.63	1.81	-0.18
4-Ethoxyphenylacetate	1.95	2.54	-0.59
4-Ethylaniline	1.96	2.1	-0.14
4-Ethylbenzenesulfonamide	1.31	1.24	0.07
4-Ethylbenzylidene t-butylamine N-oxide	2.19	2.1	0.09
4-Ethylphenol	2.5	2.61	-0.11
4-Ethylphenyl N-methylcarbamate	2.23	2.23	0.00
4-Ethylphenylacetate	2.56	2.96	-0.40
4-Ethylpyridine	1.65	1.66	-0.01
4-Ethyltoluene	3.63	3.53	0.10
4-Fluoroacetanilide	1.47	1.5	-0.03
4-Fluoroaniline	1.46	1.34	0.12
4-Fluorobenzamide	0.91	0.58	0.33
4-Fluorobenzoic acid	1.67	1.47	0.20
4-Fluorobenzylidene t-butylamine N-oxide	1.42	1.34	0.08
4-Fluoronitrobenzene	1.99	2.12	-0.13
4-Fluorophenol	1.79	1.85	-0.06
4-Fluorophenoxyacetic acid	1.41	1.49	-0.08
4-Fluorophenyl N-methylcarbamate	1.28	1.47	-0.19
4-Fluorophenylacetic acid	1.55	1.91	-0.36
4-Fluorothiophenol	2.92	2.22	0.70
4-Formylphenoxyacetic acid	0.79	0.81	-0.02
4-Heptanol	2.22	2.17	0.05
4-Heptanone	1.91	2.17	-0.26
4-Heptyn-2-ol	1.18	1.69	-0.51
4-Heptyn-3-ol	1.73	1.69	0.04

4-Hexylpyridine	3.84	3.42	0.42
4-Hexylresorcinol	3.45	3.97	-0.52
4-Hexyn-3-ol	1.2	1.25	-0.05
4-Hydroxy-3-methoxybenzaldehyde	0.97	1.1	-0.13
4-Hydroxybenzamide	0.25	0.16	0.09
4-Hydroxybenzenesulfonamide	0.06	0.06	0.00
4-Hydroxybenzoic acid heptylester	4.83	4.01	0.82
4-Hydroxybenzonitrile	1.6	1.2	0.40
4-Hydroxybenzylalcohol	0.25	0.84	-0.59
4-Hydroxy-beta-nitrostyrene	2.12	1.81	0.31
4-Hydroxybiphenyl	3.2	3.47	-0.27
4-Hydroxy-N-Nitrosopiperidine	-0.89	-0.5	-0.39
4-Hydroxyphenoxyacetic acid	0.65	1.07	-0.42
4-Hydroxyphenylacetic acid	1.96	1.49	0.47
4'-Hydroxypropiophenone	2.03	1.75	0.28
4-Iodoacetanilide	2.46	2.49	-0.03
4-Iodoaniline	2.34	2.33	0.01
4-Iodobenzamide	1.99	1.57	0.42
4-Iodobenzoic acid	3.02	2.46	0.56
4-Iodophenol	2.9	2.84	0.06
4-Iodophenoxyacetic acid	2.64	2.48	0.16
4-Iodophenyl N-methylcarbamate	2.46	2.46	0.00
4-Isopropyl-3-methylphenyl N-methylcarbamate	3.11	2.85	0.26
4-Isopropylaniline	2.47	2.38	0.09
4-Isopropylbenzamide	2.14	1.62	0.52
4-Isopropylphenoxyacetic acid	2.69	2.53	0.16
4-Isothiocyanatobenzophenone	4.88	3.96	0.92
4-Isothiocyanatodiphenylamine	4.94	4.49	0.45
4-Isothiocyanatodiphenylether	4.75	4.81	-0.06
4-Isothiocyanatophenylbenzoate	4.9	4.43	0.47
4-Methoxyacetanilide	1.14	1.41	-0.27
4-Methoxyaniline	0.95	1.25	-0.30
4-Methoxybenzaldehyde	1.59	1.5	0.09
4-Methoxybenzamide	0.86	0.49	0.37
4-Methoxybenzoic acid	1.96	1.38	0.58
4-Methoxybenzylidene t-butylamine N-oxide	1.21	1.25	-0.04
4-Methoxy-beta-nitrostyrene	2.2	2.14	0.06
4-Methoxycarbonylphenyl N-methylcarbamate	1.5	1	0.50
4-Methoxyformanilide	1.03	1.2	-0.17
4-Methoxy-N,N-dimethylaniline	1.42	1.85	-0.43
4-Methoxyphenol	1.34	1.76	-0.42
4-Methoxyphenoxyacetic acid	1.23	1.4	-0.17

4-Methoxyphenyl N,N-dimethylcarbamate	1.53	1.72	-0.19
4-Methoxyphenyl N-methylcarbamate	1.2	1.38	-0.18
4-Methoxyphenylacetate	1.54	2.11	-0.57
4-Methoxyphenylacetic acid	1.42	1.82	-0.40
4-Methoxytoluene	2.81	2.5	0.31
4-Methyl-1-heptyn-3-ol	2.13	1.67	0.46
4-Methyl-1H-pyrazole	0.9	1.46	-0.56
4-Methyl-1-pentyn-3-ol	1.07	0.79	0.28
4-Methyl-2-nitroaniline	1.82	2.04	-0.22
4-Methyl-2-pentanol	1.53	1.57	-0.04
4-Methyl-5-methoxy-8-quinolinol	2.75	2.15	0.60
4-Methyl-8-quinolinol	2.36	2.22	0.14
4-Methylacetophenone	2.28	2.05	0.23
4-Methylbenzenesulfonamide	0.82	0.8	0.02
4-Methylbenzoic acid	2.27	1.79	0.48
4-Methylbenzylalcohol	1.59	1.58	0.01
4-Methylbenzylidene t-butylamine N-oxide	1.74	1.66	0.08
4-Methyl-beta-nitrostyrene	2.66	2.55	0.11
4-Methylcyclohexanone	1.38	1.79	-0.41
4-Methyldibenzothiophene	4.8	4.85	-0.05
4-Methylformanilide	1.61	1.61	0.00
4-Methyl-N-nitrosopiperazine	0.2	-0.57	0.77
4-Methyl-N-nitrosopiperidine	1.05	1.08	-0.03
4-Methylphenoxyacetic acid	1.86	1.81	0.05
4-Methylphenylacetic acid	1.86	2.23	-0.37
4-Methylphenylisothiocyanate	3.92	3.52	0.40
4-Methylpyridine	1.22	1.22	0.00
4-Methylstyrene	3.35	3.31	0.04
4-Methylsulfonylbenzoic acid	0.67	0.44	0.23
4-Methylumbelliferon	1.58	2.47	-0.89
4-Methylvaleronitrile	1.54	1.9	-0.36
4-Nitroacetanilide	1.66	1.35	0.31
4-Nitroacetophenone	1.49	1.58	-0.09
4-Nitroaniline	1.37	1.19	0.18
4-Nitroanisole	2.03	2.03	0.00
4-Nitrobenzaldehyde	1.56	1.44	0.12
4-Nitrobenzamide	0.82	0.43	0.39
4-Nitrobenzenesulfonamide	0.64	0.33	0.31
4-Nitrobenzoic acid	1.89	1.32	0.57
4-Nitrobenzonitrile	1.19	1.47	-0.28
4-Nitrobenzylalcohol	1.26	1.11	0.15
4-Nitroformanilide	1.43	1.14	0.29

4-Nitrophenetole	2.53	2.46	0.07
4-Nitrophenol	1.91	1.7	0.21
4-Nitrophenoxyacetic acid	1.48	1.34	0.14
4-Nitrophenyl N-methylcarbamate	1.47	1.32	0.15
4-Nitrophenylacetate	1.49	2.05	-0.56
4-Nitrophenylacetic acid	1.39	1.76	-0.37
4-Nitrophenylisothiocyanate	3.62	3.05	0.57
4-Nitrophthalic acid	1	0.39	0.61
4-Nitropyrazole	0.59	0.52	0.07
4-Nitropyridine	0.48	0.75	-0.27
4-Nitroquinoline	2.06	2.15	-0.09
4-Nitroquinoline-1-oxide	1.02	0.76	0.26
4-Nitrotoluene	2.42	2.44	-0.02
4-Nonylphenol	4.48	5.69	-1.21
4-Octanol	2.68	2.61	0.07
4-Octylphenol	4.12	5.25	-1.13
4-Pentoxyphenol	3.26	3.51	-0.25
4-Pentylpyrazole	2.96	3.22	-0.26
4-Pentyn-2-ol	0.12	0.51	-0.39
4-Phenoxybenzoic acid	3.21	3.08	0.13
4-Phenyl-1-butanol	2.35	2.56	-0.21
4-Phenylbut-3-en-2-one	2.07	2.19	-0.12
4-Phenylbutylamine	2.39	2.47	-0.08
4-Phenylbutyramide	1.41	1.88	-0.47
4-Phenylbutyric acid	2.42	2.77	-0.35
4-Phenylbutyric acid methylester	2.77	3.1	-0.33
4-Phenylbutyronitrile	2.21	2.92	-0.71
4-Phenyl-N-nitrosopiperidine	2.59	2.38	0.21
4-Phenylpyridine	2.45	2.52	-0.07
4-Phenyltoluene	4.63	4.47	0.16
4-Propionylphenyl N-methylcarbamate	1.55	1.37	0.18
4-Propoylpyridine	0.77	0.8	-0.03
4-Propylbenzenesulfonamide	1.64	1.68	-0.04
4-Propylphenol	3.2	3.05	0.15
4-Propylpyridine	2.1	2.1	0.00
4-Pyridinemethanamine	-0.38	-0.2	-0.18
4-Pyridinemethanol	0.06	-0.11	0.17
4-Quinolone	0.58	1.27	-0.69
4-s-Butylphenoxyacetic acid	3.12	2.97	0.15
4-s-Butylphenyl N-methylcarbamate	3.2	2.95	0.25
4-Sulfamidobenzoic acid propylester	1.75	0.88	0.87
4-t-Butyl-3-methylphenyl N-methylcarbamate	3.38	3.21	0.17

4-t-Butyl-N-nitrosopiperidine	1.96	2.16	-0.20
4-t-Butylphenol	3.31	3.25	0.06
4-t-Butylphenyl N-methylcarbamate	3.06	2.87	0.19
4-t-Butyltoluene	5.17	4.21	0.96
4-Thiocresol	3.27	2.54	0.73
4-Tolyl N-methylcarbamate	1.66	1.79	-0.13
4-Tolylacetate	2.11	2.52	-0.41
4-Trifluoromethylaniline	1.95	2.25	-0.30
4-Trifluoromethylbenzamide	1.71	1.49	0.22
4-Trifluoromethylphenylacetic acid	2.45	2.82	-0.37
5-(2-Pyridyl)pentamide	0.39	1.01	-0.62
5-(2-Pyridyl)pentanol	1.28	1.69	-0.41
5-(2-Pyridyl)pentylamine	1.32	1.6	-0.28
5-(3-Pyridyl)pentamide	0.4	0.97	-0.57
5-(3-Pyridyl)pentanol	1.41	1.65	-0.24
5-(3-Pyridyl)pentylamine	1.41	1.56	-0.15
5-(4-Pyridyl)pentamide	0.42	0.97	-0.55
5-(4-Pyridyl)pentanol	1.39	1.65	-0.26
5-(4-Pyridyl)pentylamine	1.4	1.56	-0.16
5,5-Diphenylhydantoin	2.47	2.42	0.05
5,6-Dibromo-2-trifluoromethylbenzimidazole	4.15	3.72	0.43
5,6-Dichloro-2-trifluoromethylbenzimidazole	3.99	3.48	0.51
5,6-Dichlorovanillin	2.47	2.16	0.31
5,6-Dimethylbenzimidazole	2.35	1.94	0.41
5,8-Dihydroxy-4-methylquinoline	1.59	1.82	-0.23
5-Allyl-5-butylbarbituric acid	1.35	1.54	-0.19
5-Allyl-5-ethylbarbituric acid	0.95	0.66	0.29
5-Amino-1-pentanol	-0.53	-0.16	-0.37
5-Aminoquinoline	1.16	1.37	-0.21
5-Amyl-5-ethylbarbituric acid	2.24	1.76	0.48
5-Azauracil	-1.87	-0.85	-1.02
5-Bromo-2-trifluoromethylbenzimidazole	3.57	3.07	0.50
5-Bromoindole	3	2.78	0.22
5-Bromopentyl acetate	2.15	2.37	-0.22
5-Bromosalicylic acid	2.87	2.21	0.66
5-Bromouracil	-0.21	0.03	-0.24
5-Bromovaleric acid	1.21	1.61	-0.40
5-Bromovaleronitrile	1.05	1.76	-0.71
5-Butyl-N-methylbarbituric acid	1.1	0.41	0.69
5-Chloro-1-phenyltetrazole	1.48	1.99	-0.51
5-Chloro-2-methylthiobenzimidazole	3.22	2.73	0.49
5-Chloro-2-trifluoromethylbenzimidazole	3.39	2.95	0.44

5-Chloro-6-nitro-2-trifluoromethylbenzimidazole	3.21	2.82	0.39
5-Chloropentylacetate	2.01	2.29	-0.28
5-Chloroquinoxaline	1.75	1.86	-0.11
5-Chlorouracil	-0.35	-0.1	-0.25
5-Chlorovaleric acid	1.07	1.53	-0.46
5-Chlorovaleronitrile	0.91	1.68	-0.77
5-Chlorovanillin	1.76	1.63	0.13
5-Dimethylamino-1,3,6-trimethyluracil	0.99	0.29	0.70
5-Formyluracil	-1.03	-1.26	0.23
5-Hexyn-2-one	0.58	0.95	-0.37
5-Hexyn-3-ol	0.65	0.95	-0.30
5-Methoxy-8-quinolinol	2.06	1.81	0.25
5-Methoxyindole	2.06	2.06	0.00
5-Methyl-1-hexyn-3-ol	1.6	1.23	0.37
5-Methyl-4-nitroquinoline-1-oxide	1.36	1.1	0.26
5-Methyl-5-hexen-2-one	1.29	1.92	-0.63
5-Methyl-8-quinolinol	2.37	2.22	0.15
5-Methylindole	2.68	2.47	0.21
5-Methylquinoxaline	2.04	1.67	0.37
5-Methyluracil	-0.62	-0.26	-0.36
5-Nitro-2-trifluoromethylbenzimidazole	2.68	2.29	0.39
5-Nitroimidazole	-0.16	0.41	-0.57
5-Nitroquinoline	1.86	2.15	-0.29
5-Nitroquinoline-1-oxide	0.49	0.76	-0.27
5-Nitrosalicylic acid	2.34	1.43	0.91
5-Nonanone	2.88	3.05	-0.17
5-Octyn-3-ol	1.71	2.13	-0.42
5-Phenyl-2-pentanone	2.42	3.03	-0.61
5-Phenylvaleric acid	2.92	3.21	-0.29
5-t-Butyl-3-methylphenyl N-methylcarbamate	3.35	3.21	0.14
5-t-Butyl-4-hydroxy-2-methylacetanilide	2.67	2.84	-0.17
6,7-Dimethyl-1,4-naphthoquinone	2.49	1.81	0.68
6-Amino-1-hexanol	-0.01	0.28	-0.29
6-Aminopurine	-0.09	-0.35	0.26
6-Aminoquinoline	1.28	1.37	-0.09
6-Azaauracil	-0.59	-0.2	-0.39
6-Bromo-1-hexanol	1.73	1.84	-0.11
6-Bromohexanoic acid	1.74	2.05	-0.31
6-Bromoquinoline	2.83	2.93	-0.10
6-Chloro-1-hexanol	1.59	1.76	-0.17
6-Chloro-1-methyl-4-phenylquinazolin-2-one	2.38	3.06	-0.68
6-Chloro-4-nitroquinoline-1-oxide	1.41	1.29	0.12

6-Chloroquinoline	2.73	2.81	-0.08
6-Chloroquinoxaline	2.1	1.86	0.24
6-Chlorovanillin	1.76	1.63	0.13
6-Cyanoquinoxaline	1.01	0.7	0.31
6-Fluoro-1-methyl-4-phenylquinazolin-2-one	1.87	2.55	-0.68
6-Hydroxy-1-methyl-4-phenylquinazolin-2-one	1.72	2.13	-0.41
6-Isopropyl-3-methylphenyl N-methylcarbamate	2.84	2.85	-0.01
6-Mercaptopurine	-0.18	0.19	-0.37
6-Methoxyquinoline	2.2	2.21	-0.01
6-Methyl-1,4-naphthoquinone	2.1	1.47	0.63
6-Methyl-4-nitroquinoline-1-oxide	1.43	1.1	0.33
6-Methylquinoline	2.57	2.62	-0.05
6-Nitroquinoline	1.84	2.15	-0.31
6-Nitroquinoline-1-oxide	0.39	0.76	-0.37
6-t-Butyl-3-methylphenyl N-methylcarbamate	3.14	3.21	-0.07
7,12-Dimethylbenz[a]anthracene	5.8	6.31	-0.51
7-Azaindole	1.82	1.62	0.20
7-Bromoheptanenitrile	2.1	2.64	-0.54
7-Bromoquinoline	2.92	2.93	-0.01
7-Chloro-1-methyl-4-phenylquinazolin-2-one	2.36	3.06	-0.70
7-Chloroheptanonitrile	1.96	2.56	-0.60
7-Dimethylaminoquinoline	2.71	1.97	0.74
7-Methoxyquinoline	2.37	2.21	0.16
7-Methyl-4-nitroquinoline-1-oxide	1.42	1.1	0.32
7-Methylquinoline	2.47	2.62	-0.15
7-Nitroquinoline	1.82	2.15	-0.33
7-Nitroquinoline-1-oxide	0.36	0.76	-0.40
7-Tridecanone	5.08	4.81	0.27
7-Trifluoromethylquinoline	3.02	3.21	-0.19
8-Aminoquinoline	1.79	1.37	0.42
8-Bromo-1-octanol	2.79	2.72	0.07
8-Bromooctanoic acid	2.79	2.93	-0.14
8-Chloro-1-octanol	2.65	2.64	0.01
8-Chloroquinoline	2.33	2.81	-0.48
8-Fluoro-4-nitroquinoline-1-oxide	1	0.78	0.22
8-Methoxyquinoline	1.84	2.21	-0.37
8-Methyl-4-nitroquinoline-1-oxide	1.59	1.1	0.49
8-Methylquinoline	2.6	2.62	-0.02
8-Nitroquinoline	1.4	2.15	-0.75
8-Nitroquinoline-1-oxide	0.04	0.76	-0.72
8-Quinolinol	2	1.88	0.12
8-Sulfonamidoquinoline	0.36	1.02	-0.66

8-Trifluoromethylquinoline	2.5	3.21	-0.71
9-(1-(hydroxymethyl)butyl)adenine	0.66	0.34	0.32
9,10-Benzophenanthrene	5.49	5.59	-0.10
9,10-Dihydroanthracene	4.25	5.17	-0.92
9,10-Dimethylantracene	5.69	5.23	0.46
9-Acetylcarbazole	3.45	2.98	0.47
9-Acridinamine	2.74	2.77	-0.03
9-Anthracenol	3.61	3.83	-0.22
9-Butyladenine	1.25	1.24	0.01
9H-Fluoren-9-imine	2.43	3.09	-0.66
9H-Fluoren-9-one	3.58	3.15	0.43
9-Methylantracene	5.07	4.87	0.20
9-Pentyladenine	1.79	1.68	0.11
9-Propyladenine	0.74	0.8	-0.06
Abstral	4.05	4.53	-0.48
Accuretic	-0.03	0.06	-0.09
Acebutolol	1.77	1.31	0.46
Acenaphthene	3.92	4.35	-0.43
Acenaphthylene	4.03	4.09	-0.06
Acetaldehyde	0.45	0.27	0.18
Acetamide	-1.26	-0.74	-0.52
Acetanilide	1.16	1.48	-0.32
Acethydrazide	-1.58	-1.03	-0.55
Acetic acid	-0.17	0.15	-0.32
Acetone oxime	0.12	0.14	-0.02
Acetonitrile	-0.34	0.3	-0.64
Acetonylacetone	-0.27	0.43	-0.70
Acetophenone	1.63	1.71	-0.08
Acetylacetone	0.4	-0.01	0.41
Acetylsulfanilamide	-0.96	-0.29	-0.67
Acetylthiobenzene	2.23	2.32	-0.09
Aciclovir	-1.56	-1.43	-0.13
Acrylamide	-0.67	-0.52	-0.15
Acrylic acid	0.35	0.37	-0.02
Acticin	6.5	6.58	-0.08
Actidione	0.55	0.86	-0.31
Actiprofen	3.51	3.67	-0.16
Acular	2.1	2.76	-0.66
Adazine	5.19	5.39	-0.20
Adrucil	-0.95	-0.92	-0.03
Akineton	4.25	4.54	-0.29
Alachlor	3.52	3.11	0.41

Alclofenac	2.47	3	-0.53
Aldosterone	1.08	1.37	-0.29
Aldrin	6.5	6.25	0.25
Allobarbitol	1.07	0.88	0.19
Allyl alcohol	0.17	0.16	0.01
Allyl bromide	1.79	1.63	0.16
Allyl butyrate	1.81	2.01	-0.20
Allyl chloride	1.69	1.55	0.14
Allyl cyanide	0.4	0.96	-0.56
Allyl heptanoate	3.4	3.33	0.07
Allyl hexanoate	2.87	2.89	-0.02
Allyl phenyl ether	2.94	2.81	0.13
Allyl propanoate	1.28	1.57	-0.29
Allylamine	0.07	0.07	0.00
Allylethylamine	0.81	1.03	-0.22
Allylisopropylacetamide	1.14	1.62	-0.48
Allylpropylamine	1.33	1.47	-0.14
alpha,alpha-Dimethylphenethylamine	1.9	2.42	-0.52
alpha-Chloroisovalerylurea	1	0.78	0.22
alpha-D-Arabinopyranose	-3.02	-2.42	-0.60
alpha-Estradiol	4.01	4.23	-0.22
alpha-Hydroxybenzylpenicillin	1.4	0.6	0.80
alpha-Hydroxybutyric acid	-0.36	-0.27	-0.09
alpha-Ionone	3.85	3.5	0.35
alpha-Methyl benzylamine	1.4	1.58	-0.18
alpha-Methylstyrene	3.48	3.38	0.10
alpha-Pinene	4.44	3.98	0.46
alpha-Terpinene	4.25	4.17	0.08
Alprazolam	4.9	4.97	-0.07
Alprenolol	3.1	2.7	0.40
Ametryn	2.98	3.16	-0.18
Aminocarb	1.9	1.48	0.42
Aminopyrazine	-0.07	-0.54	0.47
Aminopyrine	0.85	0.94	-0.09
Amlodipine	3.74	3.46	0.28
Amoxicillin	-1.71	-2.01	0.30
Ampicillin	-2.17	-1.61	-0.56
Amyl acetate	2.3	2.23	0.07
Amyl formate	1.79	1.69	0.10
Amyl propionate	2.83	2.67	0.16
Amylamine	1.49	1.17	0.32
Amylbenzene	4.9	4.55	0.35

Amylisoithiocyanate	3.48	3.55	-0.07
Amylobarbitone	2.07	1.6	0.47
Anabesine	0.97	1.13	-0.16
Aniline	0.94	1.32	-0.38
Anise alcohol	1.1	1.17	-0.07
Anisole	2.11	2.16	-0.05
Anthracene	4.5	4.51	-0.01
Antipyrine	0.23	0.87	-0.64
Aprobarbital	1.37	0.94	0.43
Arabinose	-3.02	-2.93	-0.09
Arabinosylhypoxanthine	-2.08	-2.24	0.16
Arbutin	-1.35	-0.52	-0.83
Arformoterol	1.91	1.99	-0.08
Aspartic acid	-3.7	-3.09	-0.61
Aspirin	1.23	1.91	-0.68
Astemizole	5.8	5.73	0.07
Atenolol	0.16	0.47	-0.31
Atomoxetine	3.7	4.13	-0.43
Atrazine	2.61	2.61	0.00
Azanidazole	0.85	0.12	0.73
Azatadine	3.59	4.47	-0.88
Azathioprine	1.07	1.05	0.02
Azulene	3.2	3.57	-0.37
Azulfidine	3.61	3.29	0.32
Baclofen	-0.96	-0.33	-0.63
Bactrim	0.88	1.4	-0.52
Banzel	0.9	0.26	0.64
Barbital	0.65	0.44	0.21
Barbituric acid	-1.44	-1.08	-0.36
Bayleton	3.26	3.57	-0.31
BCNU	1.53	1.37	0.16
Benadryl	3.27	3.6	-0.33
Benalaxyl	3.4	3.98	-0.58
Bendroflumethiazide	1.19	1.62	-0.43
Benefin	5.29	4.57	0.72
Benomyl	2.12	2.39	-0.27
Benorylate	2.15	2.68	-0.53
Bensulfuron-methyl	2.45	2.21	0.24
Bentazone	2.83	2.69	0.14
Benz[a]anthracene	5.79	5.59	0.20
Benz[e]acephenanthrylene	5.78	6.41	-0.63
Benzalacetophenone	3.08	3.49	-0.41

Benzalcyanoacetamide	1.5	0.48	1.02
Benzaldehyde	1.48	1.57	-0.09
Benzalmalonodiamide	-0.13	-0.56	0.43
Benzalmalonodinitrile	2.12	1.52	0.60
Benzamide	0.64	0.56	0.08
Benzanilide	2.7	2.78	-0.08
Benzedrine	1.76	2.02	-0.26
Benzene	2.13	2.35	-0.22
Benzenecarbothioamide	1.49	0.89	0.60
Benzenesulfonamide	0.31	0.46	-0.15
Benzenethiol	2.52	2.2	0.32
Benzimidazole	1.32	1.26	0.06
Benzimidazole-2-thione	1.66	1.68	-0.02
Benzo[a]fluorene	5.68	5.79	-0.11
Benzo[a]naphthacene	6.81	6.67	0.14
Benzo[a]phenanthrene	5.73	5.59	0.14
Benzo[a]pyrene	5.97	6.13	-0.16
Benzo[b]fluorene	5.77	5.79	-0.02
Benzo[b]furan	2.67	2.67	0.00
Benzo[b]triphenylene	6.17	6.67	-0.50
Benzo[e]pyrene	6.44	6.13	0.31
Benzo[f]quinoline	3.25	3.28	-0.03
Benzo[g,h,i]perylene	6.63	6.67	-0.04
Benzo[ghi]fluoranthene	5.78	5.73	0.05
Benzo[j]fluoranthene	6.4	6.41	-0.01
Benzo[k]fluoranthene	6.11	6.41	-0.30
Benzohydroxamic acid	0.26	0.14	0.12
Benzoic acid	1.87	1.45	0.42
Benzonitrile	1.56	1.6	-0.04
Benzophenone	3.18	3.01	0.17
Benzothiazole	2.02	1.95	0.07
Benzotrifluoride	3.01	3.16	-0.15
Benzoylhydrazine	0.19	0.27	-0.08
Benzyl acetate	1.96	2.21	-0.25
Benzyl benzoate	3.97	3.51	0.46
Benzyl butyl phthalate	4.59	4.37	0.22
Benzyl ethyl ether	2.16	2.43	-0.27
Benzyl methyl ether	1.35	2	-0.65
Benzylamine	1.09	1.15	-0.06
Benzylaniline	3.13	3.43	-0.30
Benzylisothiocyanate	2.83	3.53	-0.70
Benzylmethylaniline	1.52	1.56	-0.04

Benzylpenicillin	1.83	1.9	-0.07
Benzylphenylether	3.79	3.89	-0.10
Benzylthiocyanate	1.99	2.36	-0.37
beta-Ethyl-beta-nitrostyrene	2.86	2.96	-0.10
beta-HCH	3.78	4.03	-0.25
beta-Ionone	3.84	3.63	0.21
Betamethasone	2.06	1.91	0.15
beta-Nitrostyrene	2.24	2.21	0.03
beta-Resorcylic acid	1.44	1.16	0.28
Bevantolol	3	3.21	-0.21
Bifenox	4.48	4.34	0.14
Bifonazole	4.77	4.43	0.34
Biphenyl	4.01	4.11	-0.10
Bis(2-chloroethyl) ether	1.29	1.25	0.04
Bis(2-hydroxyethyl)methylamine	-1.04	-1.18	0.14
Bisoprolol	2.15	2.23	-0.08
Bisphenol A	3.42	4.15	-0.73
Bitertanol	4.16	4.32	-0.16
Bornyl acetate	4.3	3.38	0.92
Bremazocine	3.2	4.13	-0.93
Brethine	1.4	1.28	0.12
Bromacil	2.11	2.45	-0.34
Bromazepam	1.65	1.64	0.01
Bromoacetamide	-0.52	-0.6	0.08
Bromoacetic acid	0.41	0.29	0.12
Bromoacetonitrile	0.36	0.44	-0.08
Bromobenzene	2.99	2.88	0.11
Bromocyclohexane	3.2	2.9	0.30
Bromoethane	1.61	1.41	0.20
Bromoperidol	3.65	3.91	-0.26
Bromophos	5.21	4.83	0.38
Bromophos-ethyl	6.15	5.69	0.46
Broxuridine	-0.29	-0.83	0.54
Budeprion	3.21	3.04	0.17
Bufexamac	1.47	1.82	-0.35
Bumetanide	1.96	2.09	-0.13
Bunitrolol	1.91	1.47	0.44
Bunolol	2.4	2.42	-0.02
Bupirimate	2.7	2.73	-0.03
Bupranolol	2.97	3.48	-0.51
Buspirone	2.3	1.61	0.69
Butachlor	4.5	4.8	-0.30

Butanal	0.88	1.15	-0.27
Butanamide	-0.21	0.14	-0.35
Butane	2.89	2.51	0.38
Butanedioic acid	-0.59	-0.24	-0.35
Butanoic acid	0.79	1.03	-0.24
Butanoic anhydride	1.39	2.26	-0.87
Butobarbitone	1.73	1.32	0.41
Butralin	4.54	4.67	-0.13
Butyl 4-hydroxybenzoate	3.57	2.69	0.88
Butyl butanoate	2.83	2.67	0.16
Butyl propanoate	2.3	2.23	0.07
Butyl thiocyanate	2.03	1.94	0.09
Butyl-1,2-dinitrate	2.36	2.76	-0.40
Butylate	4.15	3.79	0.36
Butylbenzene	4.26	4.09	0.17
Butylcellosolve	0.83	0.68	0.15
Butyldimethylamine	1.7	1.55	0.15
Butylisothiocyanate	2.92	3.11	-0.19
Butylmethylamine	1.33	1.14	0.19
Butylmethylketone	1.38	1.73	-0.35
Butylnitrate	2.15	2.23	-0.08
Butylpropylamine	2.12	2.13	-0.01
Butyranilide	2.05	2.36	-0.31
Butyric acid hydrazide	-0.62	-0.15	-0.47
Butyric acid methylester	1.29	1.36	-0.07
Butyronitrile	0.6	1.18	-0.58
Butyrophenone	2.77	2.59	0.18
Caffeine	-0.07	-0.29	0.22
Camphene	4.22	4.02	0.20
Camphorquinone	1.52	1.53	-0.01
Capraldehyde	4.01	3.79	0.22
Caproic aldehyde	1.78	2.03	-0.25
Caprolactone	0.31	1.43	-1.12
Caprylene	4.57	3.85	0.72
Caprylic aldehyde	2.95	2.91	0.04
Caprylonitrile	2.75	2.94	-0.19
Captopril	1.02	0.68	0.34
Carazolol	3.73	3.15	0.58
Carbamazepine	2.45	2.9	-0.45
Carbaril	2.36	2.45	-0.09
Carbazole	3.72	3.68	0.04
Carbendazim	1.52	1.45	0.07

Carbenicillin	1.13	1.42	-0.29
Carbofuran	2.32	2.45	-0.13
Carbophenothion	5.33	5.33	0.00
Carbophos	2.36	2.54	-0.18
Carbostyryl	1.26	1.76	-0.50
Carbromal	1.54	1.11	0.43
Carbutamide	1.01	1.34	-0.33
Carfecillin	2.96	3.6	-0.64
Carvedilol	4.14	3.97	0.17
Carvone	2.71	2.71	0.00
Cathine	0.67	0.72	-0.05
Cefacetrile	-0.45	-0.38	-0.07
Cefaclor	-1.79	-1.1	-0.69
Cefixime	0.11	0.03	0.08
Cefmetazole	-0.6	-0.97	0.37
Cefobid	-0.74	-1.06	0.32
Cefuroxime	-0.16	0	-0.16
Celebrex	3.9	4.17	-0.27
Celiprolol	1.92	1.97	-0.05
Cephamandole	0.5	-0.03	0.53
Cetamolol	1.36	0.71	0.65
Cetane	8.86	8.87	-0.01
Chloral	0.99	1.6	-0.61
Chloral hydrate	0.99	0.65	0.34
Chloramben	1.11	1.6	-0.49
Chlorazine	3.24	3.96	-0.72
Chlorbromuron	3.09	3.12	-0.03
Chlordane	6.2	6.25	-0.05
Chlorfenidim	1.94	2.05	-0.11
Chlorflurazole	3.49	3.48	0.01
Chlorguanide	2.53	2.39	0.14
Chlorimuron-ethyl	2.7	2.31	0.39
Chlorinate	2.68	3.13	-0.45
Chlormidazole	4.36	4.1	0.26
Chloroacetamide	-0.53	-0.68	0.15
Chloroacetic acid	0.22	0.21	0.01
Chloroacetic acid ethylester	0.94	0.97	-0.03
Chloroacetonitrile	0.45	0.36	0.09
Chloroambucil	3.7	3.68	0.02
Chlorobenzene	2.84	2.76	0.08
Chlorobutanol	2.03	1.95	0.08
Chloroethane	1.43	1.33	0.10

Chloromycetin	1.14	0.91	0.23
Chloroprene	2.03	2.28	-0.25
Chloropropham	3.51	3.14	0.37
Chloroquine	4.69	4.52	0.17
Chlorothalonil	2.9	3.09	-0.19
Chlorothiazide	-0.24	-0.85	0.61
Chloroxilenol	3.27	3.04	0.23
Chlorphenamine	3.39	3.65	-0.26
Chlorpromazine	5.19	4.99	0.20
Chlorpropamide	2.27	1.83	0.44
Chlorprothixene	6.03	5.77	0.26
Chlorpyrifos-methyl	4.31	4.62	-0.31
Chlorpyrifos	5.27	5.48	-0.21
Chlorsulfuron	1.79	1.85	-0.06
Chlortalidone	0.24	0.5	-0.26
Chlortoluron	2.41	2.39	0.02
Cimetidine	0.4	0.81	-0.41
Cinnamaldehyde	1.9	2.05	-0.15
Cinnamamide	1.41	1.04	0.37
Cinnamanilide	3.61	3.26	0.35
Cinnolin-4-one	0.82	1.74	-0.92
Cinoxate	2.29	2.48	-0.19
Ciprofloxacin	-1.08	-1.05	-0.03
cis-1,2-Cyclohexyl dinitrate	2.97	2.75	0.22
cis-1,2-Dichloroethylene	1.86	1.75	0.11
cis-1,3-Cyclohexyl dinitrate	2.66	2.75	-0.09
cis-1,3-Dichloropropene	1.76	2.32	-0.56
cis-2,4,6-Trimethyl-1,3,5-trioxane	0.67	0.82	-0.15
cis-2-Butene-1,4-diol	-0.81	-0.65	-0.16
cis-2-Hexen-1-ol	1.4	1.3	0.10
cis-Crotyl alcohol	0.34	0.42	-0.08
Clenbuterol	2.94	2.23	0.71
Cleocin	2.16	1.52	0.64
Clobazam	2.12	2.41	-0.29
Clofazimine	7.48	6.81	0.67
Clofenotane	6.91	6.98	-0.07
Clofibrate	3.65	3.44	0.21
Clofibric acid	2.57	2.68	-0.11
Clomethiazole	2.12	2.12	0.00
Clomicalm	5.19	5.23	-0.04
Clonazepam	3.02	2.7	0.32
Clonidine	1.57	2.06	-0.49

Clotiazepam	3.49	3.53	-0.04
Clotrimazole	5.2	5.02	0.18
Cloxacpen	2.43	2.92	-0.49
Clozapine	3.9	3.02	0.88
Colamine	-1.31	-1.48	0.17
Cordarone	7.8	8.31	-0.51
Coronene	6.7	7.21	-0.51
Cortexolone	2.52	2.3	0.22
Corticosterone	1.94	2.37	-0.43
Cortisol	1.61	1.26	0.35
Cortisone	1.47	1.28	0.19
Coumarin	1.39	2.46	-1.07
CPMC	1.64	1.98	-0.34
Creatinine	-1.76	-1.25	-0.51
Cromoglicic acid	1.6	1	0.60
Crotonic acid	0.72	0.63	0.09
Crotoxyphos	3.3	2.45	0.85
Cumene	3.66	3.47	0.19
Cyanazine	2.22	2.04	0.18
Cyanoethylene	0.25	0.52	-0.27
Cycloheptane	4	3.46	0.54
Cyclohexane	3.44	3.07	0.37
Cyclohexanecarboxylic acid	1.96	1.69	0.27
Cyclohexanethiol	2.68	2.53	0.15
Cyclohexanol	1.23	1.23	0.00
Cyclohexanone	0.81	1.51	-0.70
Cyclohexanone oxime	1.19	1.24	-0.05
Cyclohexene	2.86	2.67	0.19
Cyclohexylamine	1.49	1.1	0.39
Cyclooctane	4.45	3.85	0.60
Cyclooctatetraene	3.08	2.81	0.27
Cyclopentane	3	2.68	0.32
Cyclopentanone	0.38	1.21	-0.83
Cyclopropane	1.72	1.9	-0.18
Cyclopropylbenzene	3.27	3.39	-0.12
Cyclosarin	1.04	1.24	-0.20
Cymperator	6.05	6.08	-0.03
Cytarabine	-2.51	-2.94	0.43
Cytosine	-1.73	-1.04	-0.69
Daraprim	2.87	2.58	0.29
DDD	6.22	6.31	-0.09
DDE	6.96	6.52	0.44

Debrisoquine	0.85	1.57	-0.72
Decabromodiphenyl ether	9.97	10.36	-0.39
Decachlorodiphenyl ether	8.16	9.16	-1.00
Decamethylcyclopentasiloxane	8.07	8.03	0.04
Decane	5.8	5.69	0.11
Decanedioic acid	2.01	2.4	-0.39
Decyl-1,2-dinitrate	5.88	5.4	0.48
Decylbenzene	6.94	6.85	0.09
DEHP	7.6	7.15	0.45
delta-Decanolactone	2.39	3.36	-0.97
delta-HCH	4.14	4.03	0.11
Deprenyl	2.9	3.05	-0.15
Desipramine	4	4.29	-0.29
Desmethyldiazepam	2.93	2.83	0.10
Devrinol	3.36	3.75	-0.39
Dexamethasone	2.01	1.91	0.10
Dexamisole	1.94	2.46	-0.52
Dexfenfluramine	3.36	3.91	-0.55
Dexindoprofen	2.77	2.82	-0.05
Dexsotalol	-0.47	0.45	-0.92
Dialifos	4.69	4.12	0.57
Diallylamine	1.11	1.25	-0.14
Diamylamine	3.76	3.45	0.31
Dibenz[a,h]anthracene	6.5	6.67	-0.17
Dibenz[a,j]anthracene	7.11	6.67	0.44
Dibenzo[b,d]thiophene	4.38	4.51	-0.13
Dibenzo[b,e]pyridine	3.4	3.68	-0.28
Dibenzofuran	4.12	4	0.12
Dibenzo-p-dioxin	4.38	3.99	0.39
Dibenzyl ether	3.31	3.73	-0.42
Dibenzylamine	2.67	3.41	-0.74
Dibutyl adipate	3.9	4.07	-0.17
Dibutyl ether	3.21	2.89	0.32
Dibutyl phenyl phosphate	4.27	4.06	0.21
Dibutyl phthalate	4.53	3.95	0.58
Dibutyl suberate	4.96	4.95	0.01
Dibutyl succinate	3.6	3.19	0.41
Dibutylamine	2.68	2.57	0.11
Dibutylsulfide	4.02	3.76	0.26
Dibutylsulfoxide	1.85	1.24	0.61
Dichlorfenidim	2.68	2.58	0.10
Dichloroacetic acid	0.92	0.81	0.11

Dichloroacetonitrile	0.93	0.96	-0.03
Diclofop-methyl	4.8	4.96	-0.16
Dicloxacillin	2.91	3.45	-0.54
Dicyanomethane	-0.6	-0.23	-0.37
DIDP	7.7	8.91	-1.21
Diethanolamine	-1.43	-1.59	0.16
Diethion	5.07	5.11	-0.04
Diethyl 2-butylmalonate	3.02	2.59	0.43
Diethyl 3-oxopimelate	1.49	1.45	0.04
Diethyl 4-oxopimelate	1.54	1.45	0.09
Diethyl acetamidomalonate	0.34	-0.22	0.56
Diethyl adipate	1.79	2.31	-0.52
Diethyl allylmalonate	2.01	1.93	0.08
Diethyl benzylidenemalonate	3.13	2.74	0.39
Diethyl chloromalonate	1.64	1.24	0.40
Diethyl decanedioate	3.9	4.07	-0.17
Diethyl ethylmalonate	1.96	1.71	0.25
Diethyl isopropylidenemalonate	2.66	1.85	0.81
Diethyl malonate	0.96	0.99	-0.03
Diethyl methylmalonate	1.44	1.27	0.17
Diethyl oxalate	0.56	0.55	0.01
Diethyl phthalate	2.47	2.19	0.28
Diethyl pimelate	2.31	2.75	-0.44
Diethyl propylmalonate	2.49	2.15	0.34
Diethyl suberate	2.84	3.19	-0.35
Diethyl succinate	1.19	1.43	-0.24
Diethyl sulphide	1.95	2	-0.05
Diethylacetaldehyde	1.67	1.87	-0.20
Diethylacetamide	0.34	0.96	-0.62
Diethylamine	0.58	0.81	-0.23
Diethylcarbonate	1.21	0.81	0.40
Diethylene glycol dimethyl ether	-0.36	-0.01	-0.35
Diethyleneglycol	-1.98	-1.27	-0.71
Diethyleneglycol diethyl ether	0.39	0.85	-0.46
Diethylketone	0.99	1.29	-0.30
Diethylmethylamine	0.95	1.22	-0.27
Diethylstilbestrol	5.07	5.25	-0.18
Di flubenzuron	3.88	3.46	0.42
Di flunisal	4.32	3.24	1.08
Digitoxin	2.83	3.13	-0.30
Digoxin	1.26	1.58	-0.32
Dihexyl phthalate	5.8	5.71	0.09

Dihydro-2(3H)-thiophenone	0.6	0.85	-0.25
Dihydrocarvone	2.85	2.7	0.15
Diisoamyl ether	4.25	3.45	0.80
Diisobutyl phthalate	4.11	3.63	0.48
Diisobutylamine	2.94	2.25	0.69
Di-isooctyl phthalate	8	7.15	0.85
Diisopropyl ether	2	2.07	-0.07
Diisopropyl phthalate	2.83	3.13	-0.30
Diisopropylamine	1.4	1.67	-0.27
Diltiazem	2.7	2.98	-0.28
Dimethoxymethane	0	0.16	-0.16
Dimethyl brassylate	4.43	4.53	-0.10
Dimethyl carbonate	0.23	-0.05	0.28
Dimethyl glutarate	0.62	1.01	-0.39
Dimethyl malonate	-0.05	0.13	-0.18
Dimethyl phthalate	1.56	1.33	0.23
Dimethyl sebacate	2.84	3.21	-0.37
Dimethyl suberate	1.79	2.33	-0.54
Dimethyl succinate	0.35	0.57	-0.22
Dimethyl sulfide	1.77	1.44	0.33
Dimethyl-(2,2-dichlorovinyl) phosphate	1.42	1.15	0.27
Dimethylacetamide	-0.7	-0.14	-0.56
Dimethylamine	-0.38	-0.29	-0.09
Dimethylcyanamide	-0.15	0.32	-0.47
Dimethylether	0.1	0.27	-0.17
Dimpylate	3.81	3.21	0.60
Di-n-butylsulfone	1.76	1.87	-0.11
Dinitramine	4.3	3.8	0.50
Dinoseb	3.56	3.58	-0.02
Di-n-propyl phthalate	3.27	3.07	0.20
Diphenyl 2-ethylhexyl phosphate	5.73	5.71	0.02
Diphenyl ether	4.21	3.86	0.35
Diphenyl sulfide	4.45	4.37	0.08
Diphenylacetic acid	3.05	3.47	-0.42
Diphenylamine	3.5	3.54	-0.04
Diphenylmethane	4.14	4.57	-0.43
Diphenylmethanol	2.67	3.01	-0.34
Diphenylmethylamine	3.16	2.88	0.28
Diphenylnitrone	1.88	2.04	-0.16
Diphenylsulfone	2.4	2.89	-0.49
Diphenylsulfoxide	2.06	2.26	-0.20
Dipropyl ether	1.93	2.01	-0.08

Dipropyl sulfide	2.96	2.88	0.08
Dipropylamine	1.67	1.69	-0.02
Dipropylsulfoxide	0.74	0.36	0.38
Disugran	2.21	2.44	-0.23
Disulfoton	4.02	4.02	0.00
D-Lyxose	-3.02	-2.93	-0.09
DMSO	-1.35	-1.08	-0.27
Dodecamethylcyclohexasiloxane	8.87	9.49	-0.62
Dodecane	6.8	6.75	0.05
Dodecanedioic acid	3.07	3.28	-0.21
Dolasteron	2.42	2.7	-0.28
Dopa	-1.8	-1.98	0.18
Dosulepin	4.49	5.01	-0.52
D-Ribose	-2.32	-2.79	0.47
Dronabinol	6.97	6.74	0.23
Eicosane	10.39	10.99	-0.60
Elaidic acid	6.86	6.79	0.07
Emodepside	4.9	4.99	-0.09
Enalapril	0.16	0.7	-0.54
Enanthic acid	2.41	2.35	0.06
Enantholactam	0.24	0.89	-0.65
Endrin	5.2	5.33	-0.13
Enprofylline	0.33	0.92	-0.59
Ephedrine	1.13	1.13	0.00
Epichlorohydrin	0.45	0.7	-0.25
Epiquinine	3.44	2.82	0.62
Epivir	-0.93	-0.18	-0.75
epsilon-Aminocaproic acid	-1.95	-1.56	-0.39
epsilon-Caprolactam	-0.19	0.59	-0.78
epsilon-Caprothiolactam	0.75	0.92	-0.17
Eradicane	3.21	3.23	-0.02
Ergonovine	1.67	1.57	0.10
Esketamine	2.18	2.72	-0.54
Estriol	2.45	3.19	-0.74
Ethalfuralin	4.92	4.32	0.60
Ethane	1.81	1.45	0.36
Ethanol	-0.32	-0.06	-0.26
Ethene	1.13	1.27	-0.14
Ethinyl Estradiol	3.42	4.1	-0.68
Ethiofencarb	2.04	2.52	-0.48
Ethoxybenzene	2.51	2.59	-0.08
Ethyl 2,3-dibromobutanoate	2.5	2.53	-0.03

Ethyl 2,3-dibromopropionate	1.98	1.86	0.12
Ethyl 2-bromo-2-methylpropanoate	1.8	1.77	0.03
Ethyl 2-bromo-3-methylbutyrate	2.42	2.44	-0.02
Ethyl 2-bromobutyrate	2.02	2.16	-0.14
Ethyl 2-bromohexanoate	3.08	3.04	0.04
Ethyl 2-bromooctanoate	4.14	3.92	0.22
Ethyl 2-bromopropionate	1.49	1.72	-0.23
Ethyl 2-bromovalerate	2.55	2.6	-0.05
Ethyl 2-chloropropionate	1.35	1.6	-0.25
Ethyl 2-furancarboxylate	1.52	1.57	-0.05
Ethyl 2-methylbutanoate	1.59	2.07	-0.48
Ethyl 2-picolinate	0.87	0.9	-0.03
Ethyl 3-bromopropionate	1.44	1.49	-0.05
Ethyl 3-chloropropionate	1.3	1.41	-0.11
Ethyl 4-aminobenzoate	1.89	1.3	0.59
Ethyl 4-bromobutyrate	1.62	1.93	-0.31
Ethyl 4-chlorobutyrate	1.48	1.85	-0.37
Ethyl 4-hydroxybenzoate	2.43	1.81	0.62
Ethyl 4-pyridinecarboxylate	1.43	0.86	0.57
Ethyl 5-bromovalerate	2.15	2.37	-0.22
Ethyl 6-bromohexanoate	2.68	2.81	-0.13
Ethyl acetate	0.73	0.91	-0.18
Ethyl acetoacetate	0.24	0.49	-0.25
Ethyl acrylate	1.32	1.13	0.19
Ethyl amyl ether	2.46	2.45	0.01
Ethyl benzoate	2.64	2.21	0.43
Ethyl benzoylacetate	1.87	1.79	0.08
Ethyl bromoacetate	1.12	1.05	0.07
Ethyl butanoate	1.73	1.79	-0.06
Ethyl chloroformate	0.63	0.64	-0.01
Ethyl cyanoacetate	0.02	0.38	-0.36
Ethyl dodecanoate	5.71	5.31	0.40
Ethyl ether	0.89	1.13	-0.24
Ethyl formate	0.26	0.37	-0.11
Ethyl hexanoate	2.83	2.67	0.16
Ethyl iodide	2	2.08	-0.08
Ethyl isobutanoate	1.55	1.63	-0.08
Ethyl isothiocyanate	1.47	2.23	-0.76
Ethyl isovalerate	2.17	2.07	0.10
Ethyl lactate	-0.18	0.05	-0.23
Ethyl methyl ketone oxime	0.65	0.58	0.07
Ethyl nicotinate	1.32	0.86	0.46

Ethyl N-phenylcarbamate	2.3	2.14	0.16
Ethyl pentanoate	2.3	2.23	0.07
Ethyl phenylacetate	2.42	2.65	-0.23
Ethyl propanoate	1.21	1.35	-0.14
Ethyl salicylate	2.95	2.32	0.63
Ethyl thiocyanate	1.22	1.06	0.16
Ethyl trans-cinnamate	2.99	2.69	0.30
Ethyl trichloroacetate	2.39	2.24	0.15
Ethyl vanillin	1.58	1.53	0.05
Ethyl vinyl ether	1.04	1.34	-0.30
Ethylamine	-0.13	-0.15	0.02
Ethylbenzene	3.15	3.17	-0.02
Ethylcarbamate	-0.15	-0.08	-0.07
Ethylcarbamide	-0.74	-0.49	-0.25
Ethyldiisopropylamin	2.68	2.63	0.05
Ethyldimethylamine	0.7	0.67	0.03
Ethylenedichloride	1.48	1.39	0.09
Ethylenethiourea	-0.66	-0.6	-0.06
Ethylmethylanine	0.15	0.26	-0.11
Ethylnitrate	1	1.35	-0.35
Ethynylbenzene	2.53	2.39	0.14
Ethylimol	2.22	2.4	-0.18
Etofylline	-0.49	-1.07	0.58
Etoposide	1.97	1.29	0.68
Exalgin	1.07	1.37	-0.30
Exaltol	4.82	3.93	0.89
Famotidine	-0.81	-0.86	0.05
Fenarimol	3.6	3.2	0.40
Fenbufen	3.2	3.11	0.09
Fenchlorphos	5.07	4.71	0.36
Fenchone	3.52	2.69	0.83
Fenoprop	3.8	3.53	0.27
Fenoxycarb	4.3	3.68	0.62
Fenpropathrin	6	5.26	0.74
Fenpropimorph	4.93	5.07	-0.14
Fensulfothion	2.23	2.34	-0.11
Fenthion	4.09	3.93	0.16
Fenthoate	3.69	3.76	-0.07
Fenvalerate	6.2	6.61	-0.41
Fimepinostat	-1.49	-0.93	-0.56
Finasteride	3.03	3.89	-0.86
Fipronil	3.47	3.52	-0.05

Fleroxacin	-0.55	-0.16	-0.39
Floxuridine	-1.38	-1.78	0.40
Fluchloralin	4.63	4.19	0.44
Flucloxacillin	2.61	2.94	-0.33
Fluconazole	0.5	0.73	-0.23
Fludrocortisone	1.67	1.75	-0.08
Flufenamic acid	5.25	4.2	1.05
Flumazenil	1.64	1.36	0.28
Flumequine	1.72	2.22	-0.50
Flunarizine	5.78	5.74	0.04
Flunitrazepam	2.06	2.08	-0.02
Fluometuron	2.42	2.45	-0.03
Fluoranthene	5.16	5.33	-0.17
Fluorene	4.18	4.71	-0.53
Fluoroacetamide	-1.05	-1.3	0.25
Fluorobenzene	2.27	2.25	0.02
Flupentixol	4.51	5.06	-0.55
Flurbiprofen	3.99	3.83	0.16
Fluridone	2.98	3.96	-0.98
Flutamide	3.35	3	0.35
Fluvastatin	4.17	5.13	-0.96
Fomesafen	3	3.2	-0.20
Formaldehyde diethylacetal	0.84	1.02	-0.18
Formamide	-1.51	-0.95	-0.56
Formamidoxime	-1.64	-1.26	-0.38
Formanilide	1.15	1.27	-0.12
Formic acid	-0.54	-0.39	-0.15
Formylhydrazine	-2.05	-1.24	-0.81
Ftorafur	-0.27	0.12	-0.39
Furan	1.34	1.34	0.00
Furfural	0.52	0.93	-0.41
Fusaric acid	0.68	0.41	0.27
gamma-Decalactone	2.72	3.5	-0.78
gamma-Nonanolactone	1.83	3.06	-1.23
Ganciclovir	-2.07	-2.03	-0.04
Gitoxin	1.68	1.58	0.10
Glycerol trinitrate	1.62	1.98	-0.36
Glyceryltriacetate	0.25	0.66	-0.41
Glycine	-3	-3.32	0.32
Glydiazinamide	1.91	1.22	0.69
Glyme	-0.21	0.13	-0.34
Griseofulvin	2.18	2.43	-0.25

Guajen	4.4	4.15	0.25
Guanabenz	3.02	2.59	0.43
Guanidine	-1.25	-1.25	0.00
Guanine	-0.91	-0.54	-0.37
Guanosine	-1.89	-2.44	0.55
Harmalol	2.19	2.73	-0.54
Harmony	1.23	0.39	0.84
Hemimellitene	3.55	3.43	0.12
Heptachlor	5.27	6.02	-0.75
Heptachlor epoxide	5.4	5.1	0.30
Heptadecane	8.79	9.4	-0.61
Heptane	4.66	4.1	0.56
Heptanedioic acid	0.58	1.08	-0.50
Heptanonitrile	2.25	2.5	-0.25
Heptanoyl chloride	3.52	3.48	0.04
Heptyl bromide	4.36	3.61	0.75
Heptylbenzene	5.37	5.47	-0.10
Hexabromobenzene	6.07	6.13	-0.06
Hexachlorobenzene	5.73	5.41	0.32
Hexachlorobutadiene	4.78	4.77	0.01
Hexachloroethane	4.14	3.93	0.21
Hexadecanedioic acid	5.7	5.04	0.66
Hexafluoro-2-propanol	1.66	1.59	0.07
Hexafluorobenzene	2.54	2.35	0.19
Hexamethylbenzene	4.61	4.51	0.10
Hexane	3.8	3.57	0.23
Hexanenitrile	1.66	2.06	-0.40
Hexanoyl chloride	2.99	3.04	-0.05
Hexobarbital	1.49	1.14	0.35
Hexyl bromide	3.8	3.17	0.63
Hexyl-1,2-dinitrate	3.51	3.64	-0.13
Hexylbenzene	5.52	5.01	0.51
Hexylcarbamate	1.85	1.68	0.17
Hexylisothiocyanate	4.01	3.99	0.02
Hydracrylic acid	-0.62	-0.74	0.12
Hydrocinnamonitrile	1.7	2.48	-0.78
Hydrocinnamyl alcohol	1.88	2.12	-0.24
Hydrocortisone hemipimelate	3.26	3.05	0.21
Hydroflumethiazide	0.54	0.46	0.08
Hydroxyacetic acid	-1.11	-1.18	0.07
Hydroxyurea	-1.27	-1.72	0.45
Hydroxyzine	3.55	2.98	0.57

Hyoscyamine	1.83	2.3	-0.47
Hypoxanthine	-1.31	-0.34	-0.97
Imazapyr	0.22	1.05	-0.83
Imazaquin	1.86	2.45	-0.59
Imidazole	-0.08	-0.68	0.60
Imipramine	4.62	4.7	-0.08
Imiquimod	2.7	2.4	0.30
Indane	3.18	3.59	-0.41
Indene	2.92	3.47	-0.55
Indinavir	2.92	2.83	0.09
Indol-3-ylacetic acid	1.41	1.86	-0.45
Indole	2.14	2.13	0.01
Indometacin	3.1	4.03	-0.93
Iodoacetamide	-0.19	0.07	-0.26
Iodobenzene	3.25	3.24	0.01
Iohexol	-3.05	-2.04	-1.01
Iopromide	-2.05	-1.04	-1.01
Ioversol	-2.98	-2.51	-0.47
Ioxynil	3.43	3.22	0.21
Ipronidazole	1.06	1.59	-0.53
Isoamyl acetate	2.25	2.07	0.18
Isobutene	2.34	1.98	0.36
Isobutyl formate	1.19	1.09	0.10
Isobutyl isobutyrate	2.48	2.35	0.13
Isobutyl methyl ketone	1.31	1.57	-0.26
Isobutyl propanoate	2.17	2.07	0.10
Isobutylbenzene	4.54	3.93	0.61
Isobutylpropylamine	2.07	1.97	0.10
Isobutyranilide	2.02	2.2	-0.18
Isobutyronitrile	0.47	1.02	-0.55
Isocarboxazid	1.49	1.23	0.26
Isocumene	3.69	3.63	0.06
Isodecyl diphenyl phosphate	5.7	6.59	-0.89
Isohexanoic acid	1.75	1.75	0.00
Isoleucine	-1.69	-1.76	0.07
Isoleucinol	0.47	-0.33	0.80
Isoniazid	-1.14	-1.08	-0.06
Isopentyl alcohol	1.16	1.1	0.06
Isopentyl chloride	2.98	2.49	0.49
Isopentyl propionate	2.76	2.51	0.25
Isopentylamine	1.32	1.01	0.31
Isophthalamide	-0.21	-1.11	0.90

Isophthalic acid	1.66	0.52	1.14
Isoprene	2.42	2.22	0.20
Isopropanolamine	-0.96	-1.01	0.05
Isopropenylacetate	1.07	1.52	-0.45
Isopropylacetate	1.02	1.38	-0.36
Isopropylamine	0.26	0.28	-0.02
Isopropylnitrate	1.66	1.82	-0.16
Isoproturon	2.87	2.58	0.29
Isoquinoline	2.08	1.88	0.20
Isosorbide	-1.31	-1.87	0.56
Isosorbide 5-nitrate	-0.4	-0.72	0.32
Isotretinoin	6.3	5.63	0.67
Isovaleronitrile	1.12	1.46	-0.34
Isoxazole	0.08	-0.8	0.88
Isoxicam	2.83	3.56	-0.73
Kappa-bifenthrin	6.27	7.39	-1.12
Kentanserin	3.01	2.5	0.51
Kepone	5.44	5.43	0.01
Ketoconazole	4.34	3.88	0.46
Ketoprofen	3.16	2.95	0.21
Labetalol	3.09	2.74	0.35
Lacidipine	5.56	6.06	-0.50
Lactic acid	-0.72	-0.71	-0.01
Lactonitrile	-0.94	-0.56	-0.38
lambda-Cyhalothrin	7	6.54	0.46
Latamoxef	-0.58	-0.72	0.14
Lauric acid	4.2	4.55	-0.35
Lauroitrile	4.9	4.7	0.20
Lawsone	1.38	0.81	0.57
Leucine	-1.57	-1.76	0.19
Levalbuterol	1.4	1.46	-0.06
Levobetaxolol	2.81	2.98	-0.17
Levofloxacin	-0.28	0.72	-1.00
Levomoprolol	1.69	1.63	0.06
Levopropicillin	2.65	2.39	0.26
Levopropoxyphene	4.4	5.19	-0.79
Lidoflazine	5.6	6.02	-0.42
Lignocaine	2.9	2.66	0.24
Lincomycin	0.2	0.23	-0.03
Lindane	3.55	4.03	-0.48
Linuron	3.2	3	0.20
L-Menthone	3.05	2.79	0.26

Lomefloxacin	-0.8	-0.98	0.18
Lomustine	2.83	2.56	0.27
Loratadine	5.2	5.4	-0.20
Lormetazepam	2.38	3.13	-0.75
Lysine	-2.82	-3.02	0.20
Malic acid	-1.26	-1.03	-0.23
Mandelic acid	0.62	0.59	0.03
Mandelic acid ethylester	0.91	1.35	-0.44
m-Anisic acid	2.02	1.38	0.64
m-Anisidine	0.93	1.25	-0.32
m-Anthranilic acid	0.34	0.54	-0.20
MCPB	3.43	3.22	0.21
m-Cresol	1.98	2.17	-0.19
m-Cresylacetate	2.09	2.52	-0.43
m-Diacetamidobenzene	0.5	0.73	-0.23
Mebendazole	2.83	2.23	0.60
Mecoprop	3.13	2.81	0.32
Medazepam	4.05	3.54	0.51
Mefoxine	-0.02	0.39	-0.41
Meloxicam	3.01	2.81	0.20
Memantine	3.28	2.9	0.38
Menthol	3.4	2.51	0.89
Mephenamic acid	4.2	3.95	0.25
Mephenate	2.01	1.98	0.03
Mephenesin	1.41	1	0.41
Mepindolol	2.3	2.71	-0.41
Meproamate	0.7	0.53	0.17
Mepyramine	3.27	3.14	0.13
Mercaptoacetic acid	0.09	0.2	-0.11
Mercaptodimethur	2.92	2.6	0.32
Mescaline	0.78	1.38	-0.60
Mesitol	2.73	2.85	-0.12
Mesoridazine	3.05	3.74	-0.69
Metalaxyl	1.65	1.67	-0.02
Metaxone	2.69	2.34	0.35
Methadone	3.93	4.8	-0.87
Methanol	-0.77	-0.49	-0.28
Methaqualone	2.5	2.77	-0.27
Methicillin	1.3	1.83	-0.53
Methomyl	0.6	1.01	-0.41
Methotrimeprazine	4.68	4.67	0.01
Methoxychlor	5.08	5.78	-0.70

Methoxytetrachlorocyclohexane	2.99	2.99	0.00
Methyl (Z) 9-octadecenoate	7.45	7.12	0.33
Methyl 2-hydroxybenzoate	2.46	1.89	0.57
Methyl 2-methoxybenzoate	2.04	1.71	0.33
Methyl 2-methylbutyrate	1.55	1.64	-0.09
Methyl 4-hydroxybenzoate	1.96	1.38	0.58
Methyl 5-bromovalerate	1.62	1.94	-0.32
Methyl acetate	0.18	0.48	-0.30
Methyl acrylate	0.8	0.7	0.10
Methyl benzoate	2.12	1.78	0.34
Methyl carbamate	-0.66	-0.51	-0.15
Methyl cellosolve	-0.77	-0.63	-0.14
Methyl chlorocarbonate	0.14	0.21	-0.07
Methyl decanoate	4.41	4	0.41
Methyl formate	0.03	-0.06	0.09
Methyl hexanoate	2.3	2.24	0.06
Methyl hydrocinnamate	2.32	2.66	-0.34
Methyl isoamyl ketone	1.88	2.01	-0.13
Methyl isonicotinate	0.87	0.43	0.44
Methyl laurate	5.41	4.88	0.53
Methyl levulinate	-0.13	0.5	-0.63
Methyl methacrylate	1.38	1.11	0.27
Methyl nicotinate	0.81	0.43	0.38
Methyl N-methylcarbamate	-0.06	-0.25	0.19
Methyl nonanoate	3.88	3.56	0.32
Methyl octanoate	3.36	3.12	0.24
Methyl phenylacetate	1.83	2.22	-0.39
Methyl propanoate	0.84	0.92	-0.08
Methyl trans-3-pentenoate	1.28	1.4	-0.12
Methyl trans-cinnamate	2.62	2.26	0.36
Methyl trichloroacetate	2.03	1.81	0.22
Methyl trifluoroacetate	0.6	1.07	-0.47
Methyl undecanoate	4.79	4.44	0.35
Methyl valerate	1.96	1.8	0.16
Methyl Z,Z-9,12-octadecadieneoate	6.82	6.72	0.10
Methylacetamide	-1.05	-0.48	-0.57
Methylamine	-0.57	-0.7	0.13
Methylbenzene	2.73	2.71	0.02
Methylchloroacetate	0.63	0.54	0.09
Methylchloroform	2.49	2.6	-0.11
Methylcyclohexane	3.88	3.44	0.44
Methylcyclopentane	3.37	3.05	0.32

Methylenanthate	2.83	2.68	0.15
Methylhippurate	0.82	0.58	0.24
Methylhydrazine	-1.05	-1.08	0.03
Methylnitrophos	3.3	3.33	-0.03
Methyl-n-propylketone	0.91	1.29	-0.38
Methyloxiran	0.03	0.64	-0.61
Methylparathion	2.86	2.99	-0.13
Methylpentachlorocyclohexane	4.04	4.06	-0.02
Methylphenobarbital	1.84	1.19	0.65
Methylphenylsulfone	0.47	1.22	-0.75
Methylphenylsulfoxide	0.55	0.59	-0.04
Methylthiocyanate	0.73	0.78	-0.05
Methylthiopentachlorocyclohexane	3.75	4.18	-0.43
Methyltriazothion	2.75	2.79	-0.04
Metolachlor	3.13	2.96	0.17
Metolcarb	1.7	1.79	-0.09
Metoprolol	2.34	1.91	0.43
Metosulam	2.5	2.88	-0.38
Metribuzin	1.58	1.48	0.10
Metronidazol	-0.1	0.09	-0.19
Mevinphos	1.2	0.25	0.95
Mexiletine	2.15	2.28	-0.13
Midazolam	3.27	3.73	-0.46
Molinate	3.21	2.59	0.62
Monacolin K	4.26	5.36	-1.10
Monocrotophos	-0.2	-0.71	0.51
Monolinuron	2.3	2.47	-0.17
Moracizine	2.98	2.81	0.17
Morpholine	-0.86	-0.71	-0.15
MTBE	1.05	1.38	-0.33
m-Toluamide	1.18	0.9	0.28
m-Toluidine	1.4	1.66	-0.26
m-Tolyl N,N-dimethylcarbamate	2.05	2.13	-0.08
Mustard oil	1.94	2.45	-0.51
N-(2,6-dichlorophenylmethylene)benzenamine N-oxide	2.61	3.1	-0.49
N-(2-Chloroethyl)-N'-(4-hydroxycyclohexyl)-N-nitrosoarea	1.05	1.26	-0.21
N-(2-Chloroethyl)-N-nitrosoarea	0.57	0.5	0.07
N-(2-Methoxyphenyl)sulfanilamide	1.56	1.69	-0.13
N-(2-Norbornyl)-N'-(2-chloroethyl)-N'-nitrosoarea	2.98	2.74	0.24
N-(3,4-Dichlorophenyl)-N'-phenylurea	4.7	4.2	0.50
N-(3,5-Dibromo-2-pyridyl)sulfanilamide	2.74	2.55	0.19
N-(3,5-Dichloro-2-pyridyl)sulfanilamide	1.97	2.31	-0.34

N-(3-Bromo-2-pyridyl)sulfanilamide	1.24	1.9	-0.66
N-(4-Isopropylphenylmethylene)benzenamine N-oxide	3.37	3.1	0.27
N-(4-Methoxyphenyl)sulfanilamide	1.51	1.69	-0.18
N-(4-Methoxyphenylmethylene)benzenamine N-oxide	1.94	1.97	-0.03
N-(4-Methylbenzylidene)aniline N-oxide	2.41	2.38	0.03
N,N'-Diacetylurea	-0.68	-0.47	-0.21
N,N-Diallylurea	0.64	0.84	-0.20
N,N'-Dibutylurea	1.4	2.08	-0.68
N,N-Diethylaniline	3.31	3.02	0.29
N,N-Diethyl-N'-methyl-N'-nitrosourea	1.11	1.08	0.03
N,N-Dimethyl-2-anisidine	1.63	1.85	-0.22
N,N-Dimethyl-2-methoxybenzamide	0.71	1.09	-0.38
N,N-Dimethyl-3-methoxybenzamide	1	1.09	-0.09
N,N-Dimethyl-3-toluidine	2.8	2.26	0.54
N,N-Dimethyl-4-methoxybenzamide	0.96	1.09	-0.13
N,N-Dimethylaniline	2.31	1.92	0.39
N,N-Dimethylbenzamide	0.62	1.16	-0.54
N,N-Dimethylbenzenesulfonamide	1.35	0.87	0.48
N,N-Dimethylformamide	-0.74	-0.35	-0.39
N,N-Dimethyl-N'-(3-chlorophenyl)urea	2	2.05	-0.05
N,N-Dimethyl-N'-(4-bromophenyl)urea	2.19	2.17	0.02
N,N-Dimethyl-N'-(4-nitrophenyl)urea	1.51	1.39	0.12
N,N-Dimethyl-N'-(4-tolyl)urea	1.98	1.86	0.12
N,N-Dimethyl-N',N'-diphenylurea	2.8	2.88	-0.08
N,N'-Dimethyl-N-phenylurea	1.02	1.07	-0.05
N,N-Dimethylphenoxyacetamide	0.77	1.18	-0.41
N,N-Dimethylpropionamide	-0.11	0.3	-0.41
N,N-Dimethyl-p-toluidine	2.61	2.26	0.35
N,N'-Dinitrosopiperazine	-0.85	-0.93	0.08
N-Acetylanthranilic acid	1.88	1.21	0.67
Nadolol	0.71	1.5	-0.79
Nalidixic acid	1.59	1.38	0.21
Naloxone	2.09	2.12	-0.03
Naphthalene	3.35	3.43	-0.08
n-Butyl acetate	1.7	1.79	-0.09
n-Butyl acrylate	2.36	2.01	0.35
n-Butylcarbamate	0.85	0.8	0.05
n-Butylformate	1.32	1.25	0.07
n-Butylurea	0.41	0.39	0.02
N-Cyano-2-(3,3-dimethyl-1-triazenyl)-benzamide	0.8	-0.07	0.87
n-Decanoic acid	4.09	3.67	0.42
n-Decylacetate	4.94	4.43	0.51

n-Decylamine	4.1	3.37	0.73
n-Dodecanal	5.07	4.67	0.40
Nebivolol	4.04	3.49	0.55
Neburea	3.8	4.01	-0.21
Necrostatin-1	0.63	1.06	-0.43
Nedocromil	2.22	1.82	0.40
Neohexane	3.82	3.33	0.49
Neopentyl alcohol	1.36	1.02	0.34
N-Ethylaniline	2.16	2.13	0.03
N-Ethylbromoacetamide	0.34	0.21	0.13
N-Ethyl-N'-phenylurea	1.64	1.73	-0.09
Neurontin	-1.25	-0.98	-0.27
Nevirapine	2.41	2.7	-0.29
n-Heptaldehyde	1.99	2.47	-0.48
n-Heptylamine	2.57	2.05	0.52
n-Hexanoic acid	1.92	1.91	0.01
n-Hexylacetate	2.83	2.67	0.16
n-Hexylamine	2.06	1.61	0.45
n-Hexylformate	2.38	2.13	0.25
N-Hydroxyacetamide	-1.54	-1.16	-0.38
N-Hydroxy-N'-butylurea	0.32	-0.03	0.35
N-Hydroxy-N'-propylurea	-0.22	-0.47	0.25
Nicosulfuron	0.5	0.83	-0.33
Niflumic acid	4.43	3.69	0.74
Nimesulide	2.6	2.5	0.10
Nimorazole	0.07	-0.17	0.24
Ninhydrin	0.65	0.64	0.01
Nitrazepam	2.12	2.17	-0.05
Nitrobenzene	1.85	2.1	-0.25
Nitroethane	0.18	0.41	-0.23
Nitroethylene	0.01	0.65	-0.64
Nitrofungin	2.33	2.23	0.10
Nitromide	0.83	0.3	0.53
Nitrophenylmethane	1.75	1.71	0.04
N-Maleoyl-3-aminopropionic acid ethylester	0.41	-0.12	0.53
N-Methyl-2-pyrrolidone	-0.38	0.33	-0.71
N-Methyl-2-quinolone	1.45	1.65	-0.20
N-Methyl-3,5-dimethylphenyl carbamate	2.23	2.13	0.10
N-Methyl-4-nitroaniline	2.04	1.45	0.59
N-Methylaniline	1.7	1.58	0.12
N-Methylformamide	-0.97	-0.69	-0.28
N-Methylformanilide	1.09	1.16	-0.07

N-Methylmorpholine	-0.33	-0.3	-0.03
N-Methyl-N-benzylaniline	4.22	3.29	0.93
N-Methyl-N-nitrosourea	-0.1	-0.11	0.01
N-Methyl-N-phenylthiourea	0.85	0.85	0.00
N-Methyl-o-toluidine	2.16	1.92	0.24
N-Methylpiperidine	1.3	1.16	0.14
N-Methylpropargylamine	0.08	-0.08	0.16
N-Methylpropylamine	0.84	0.7	0.14
N-Methyl-p-toluidine	2.15	1.92	0.23
N-Nitroso-4-piperidone	-0.47	-0.22	-0.25
N-Nitrosodibutylamine	1.92	2.62	-0.70
N-Nitrosodiethanolamine	-1.51	-1.54	0.03
N-Nitrosodiethylamine	0.48	0.86	-0.38
N-Nitrosodiisopropylamine	1.63	1.72	-0.09
N-Nitrosodimethylamine	-0.57	-0.24	-0.33
N-Nitrosodiphenylamine	3.13	3.73	-0.60
N-Nitrosodipropylamine	1.36	1.74	-0.38
N-Nitrosomorpholine	-0.44	-0.66	0.22
N-Nitrosopiperidine	0.63	0.8	-0.17
N-Nitrosopyrrolidone	-0.19	0.41	-0.60
N-Nitrosothiomorpholine	0.4	0.21	0.19
N-Nitrosotriethylurea	1.54	1.63	-0.09
N-Nitrosotrimethylurea	0.36	-0.02	0.38
n-Nonanal	3.48	3.35	0.13
n-Nonylamine	3.57	2.93	0.64
n-Octanoic acid	3.05	2.79	0.26
n-Octylacetate	3.88	3.55	0.33
n-Octylamine	3.04	2.49	0.55
Nonane	5.65	5.16	0.49
Nonanedioic acid	1.57	1.96	-0.39
Nonylbenzene	6.41	6.39	0.02
Nopinene	4.16	4.02	0.14
Norethisterone	2.97	3.53	-0.56
Norfloxacin	-1.03	-1.4	0.37
Norflurazon	2.3	1.46	0.84
Nortriptyline	4.04	5.07	-1.03
N-Phenylanthranilic acid	4.36	3.27	1.09
N-Phenylglycine	0.62	1.01	-0.39
N-Phenylhydroxylamine	0.79	0.9	-0.11
N-Phenylmorpholine	1.36	1.5	-0.14
N-Phenylpiperidine	2.78	2.96	-0.18
N-Phenylsulfamide	0.4	0.61	-0.21

n-Propyl acetate	1.24	1.35	-0.11
n-Propyl benzoate	3.01	2.65	0.36
N-Propylaniline	2.45	2.57	-0.12
n-Propylformate	0.83	0.81	0.02
N-p-Tolylsulfanilamide	1.56	2.1	-0.54
N-Salicylideneaniline	1.55	1.35	0.20
n-Undecanoic acid	4.53	4.11	0.42
n-Undecylamine	4.63	3.81	0.82
n-Valeraldehyde	1.36	1.59	-0.23
O,O'-Diethyl-O''-(benzothien-3-yl)glyoxylonitrile oximino phosphate	0.56	0.21	0.35
O,O'-Diethyl-O''-3,4-dimethoxyphenylglyoxylonitrile oximino thiophosphate	-0.19	0.54	-0.73
O,O'-Diethyl-O''-4-chlorophenylglyoxylonitrile oximino thiophosphate	0.47	1.21	-0.74
O,O'-Diethyl-O''-4-fluorophenylglyoxylonitrile oximino thiophosphate	0.35	0.7	-0.35
O,O-Diethyl-O-phenylphosphate	1.34	2.3	-0.96
O,O'-Diisopropyl-O''-(benzothien-3-yl)glyoxylonitrile oximino phosphate	1.56	1.15	0.41
O,O'-Diisopropyl-O''-3,4-dimethoxyphenylglyoxylonitrile oximino phosphate	-0.38	-0.2	-0.18
O,O'-Diisopropyl-O''-3,4-dimethoxyphenylglyoxylonitrile oximino thiophosphate	0.47	1.48	-1.01
O,O'-Diisopropyl-O''-4-chlorophenylglyoxylonitrile oximino phosphate	-0.2	0.47	-0.67
O,O'-Diisopropyl-O''-4-fluorophenylglyoxylonitrile oximino phosphate	-0.43	-0.04	-0.39
O,O'-Diisopropyl-O''-phenylglyoxylonitrile oximino phosphate	0.06	-0.06	0.12
O,O'-Diisopropyl-O''-phenylglyoxylonitrile oximino thiophosphate	2.07	1.62	0.45
O,O'-Dimethyl-O''-(benzothien-3-yl)glyoxylonitrile oximino thiophosphate	1.94	1.03	0.91
O,O'-Dimethyl-O''-4-fluorophenylglyoxylonitrile oximino phosphate	-1.08	-1.84	0.76
O,O'-Dimethyl-O''-phenylglyoxylonitrile oximino phosphate	-1.01	-1.86	0.85
o-Anisic acid	1.59	1.89	-0.30
o-Anthranilic acid	1.26	1.05	0.21
o-Cresol	1.98	2.17	-0.19
o-Cresylacetate	2.11	2.52	-0.41
Octachlorodibenzo-p-dioxin	8.6	8.23	0.37
Octachloronaphthalene	7.7	7.47	0.23
Octachlorostyrene	6.29	6.97	-0.68
Octadecane	9.32	9.93	-0.61
Octamethylcyclotetrasiloxane	6.98	6.57	0.41
Octane	5.18	4.63	0.55

Octanedioic acid	1.14	1.52	-0.38
Octanoyl chloride	4.05	3.92	0.13
Octyl-1,2-dinitrate	4.63	4.52	0.11
Octylbenzene	6.3	5.93	0.37
Octylcyanide	3.12	3.38	-0.26
o-Cumenol	2.88	2.89	-0.01
Optipranolol	2.28	2.67	-0.39
Ornidazole	0.6	0.62	-0.02
Ornithine	-4.41	-3.46	-0.95
Orphenadrine	3.77	3.94	-0.17
o-Toluidine	1.43	1.66	-0.23
o-Tolyl N,N-dimethylcarbamate	1.86	2.13	-0.27
Oxacillin	2.38	2.39	-0.01
Oxamniquine	2.24	1.67	0.57
Oxasulfuron	1.1	0.58	0.52
Oxazepam	2.17	2.6	-0.43
Oxirane	-0.3	0.17	-0.47
Oxprenolol	2.1	2.28	-0.18
Oxycarboxin	0.74	0.62	0.12
Oxyphenbutazone	2.72	2.79	-0.07
p-Anthranilic acid	0.86	0.54	0.32
Papaverine	2.95	3.72	-0.77
Paracetamol	0.34	1.08	-0.74
Paspertin	2.62	1.93	0.69
p-Benzidine	1.34	2.05	-0.71
PBN	1.22	1.32	-0.10
PCNB	4.64	4.75	-0.11
p-Cresol	1.97	2.17	-0.20
p-Cresyl diphenyl phosphate	4.4	4.5	-0.10
p-Cymene	4.1	3.83	0.27
Pebulate	3.84	3.67	0.17
Pefloxacin	0.27	0.89	-0.62
Pelargonic acid	3.47	3.23	0.24
Penbutolol	4.15	3.68	0.47
Penconazole	3.4	4.36	-0.96
Penoxalin	5.18	4.37	0.81
Pentachloroanisole	5.45	4.81	0.64
Pentachlorobenzene	5.17	4.88	0.29
Pentachlorobenzimidazole	4.53	4.57	-0.04
Pentachloroethane	3.22	3.26	-0.04
Pentachlorophenol	5.12	4.48	0.64
Pentachloropyridine	3.53	3.77	-0.24

Pentadecane	7.72	8.34	-0.62
Pentafluorobenzene	2.53	2.33	0.20
Pentafluorothiophenol	1.56	2.3	-0.74
Pentamethylbenzene	4.56	4.15	0.41
Pentane	3.39	3.04	0.35
Pentanedioic acid	-0.29	0.2	-0.49
Pentanenitrile	1.12	1.62	-0.50
Pentanoic acid	1.39	1.47	-0.08
Pentobarbital	1.4	1.6	-0.20
Pentoxifylline	0.72	0.72	0.00
Pentyl benzoate	3.79	3.53	0.26
Pentyl-1,2-dinitrate	2.94	3.2	-0.26
Pentylcarbamate	1.35	1.24	0.11
Peonol	1.98	1.75	0.23
Perazine	3.9	4.13	-0.23
Perchlorobiphenyl	8.27	9.17	-0.90
Perchlorocyclopentadiene	5.04	4.81	0.23
Peridol	4.3	3.79	0.51
Perphenazine	4.2	3.88	0.32
Pervitin	2.07	2.43	-0.36
Perylene	5.82	6.13	-0.31
Pethidine	2.45	2.74	-0.29
Phenacemide	0.87	1.11	-0.24
Phenanthrene	4.56	4.51	0.05
Phenanthrene-9,10-dione	2.52	2.29	0.23
Phenazine	2.84	3.13	-0.29
Phenethyl acetate	2.42	2.65	-0.23
Phenethyl alcohol	1.42	1.68	-0.26
Pheneticillin	2.28	1.95	0.33
Phenindione	2.9	2.67	0.23
Phenobarbital	1.47	2.16	-0.69
Phenol	1.5	1.83	-0.33
Phenolphthalol	3.27	4.1	-0.83
Phenothiazine	3.78	4.18	-0.40
Phenoxyacetamide	0.76	0.58	0.18
Phenoxyacetic acid	1.34	1.47	-0.13
Phenoxymethylpenicillin	2.09	1.48	0.61
Phenserine	4.19	4.17	0.02
Phenyl aminosalicylate	3.15	2.68	0.47
Phenyl benzoate	3.59	3.48	0.11
Phenyl N,N-dimethylcarbamate	1.69	1.79	-0.10
Phenyl N-methylcarbamate	1.24	1.45	-0.21

Phenyl-2-tolylcarbinol	3.06	3.35	-0.29
Phenyl-4-tolylcarbinol	3.13	3.35	-0.22
Phenylacetamide	0.45	1	-0.55
Phenylacetate	1.49	2.18	-0.69
Phenylacetic acid	1.41	1.89	-0.48
Phenylacetonitrile	1.56	2.04	-0.48
Phenylalanine	-1.43	-1.18	-0.25
Phenylbutazone	3.16	3.19	-0.03
Phenylcyclopropylcarbinol	1.95	2.35	-0.40
Phenylethanal	1.78	2.01	-0.23
Phenylformate	1.26	1.64	-0.38
Phenylglycerol	0.7	-0.22	0.92
Phenylhydrazine	1.25	1.03	0.22
Phenylisocyanate	2.59	2.29	0.30
Phenylisothiocyanate	3.28	3.18	0.10
Phenylmethanol	1.1	1.24	-0.14
Phenylpropylether	3.18	3.03	0.15
Phenylthioacetic acid	1.91	1.86	0.05
Phenylthiocyanate	2.54	2.45	0.09
Phenylthiourea	0.73	0.96	-0.23
Phenyltrifluoromethylsulfone	2.68	2.6	0.08
Phenylurea	0.82	0.92	-0.10
Phenylvinylketone	1.88	1.93	-0.05
Phlorol	2.47	2.61	-0.14
Phosphamide	0.78	0.68	0.10
Phthalic acid	0.73	0.52	0.21
Phthalic anhydride	1.43	1.6	-0.17
Phthalophos	2.78	2.75	0.03
Phthiocol	1.2	1.22	-0.02
Physostigmine	1.58	2.21	-0.63
Pimozide	6.3	6.75	-0.45
Pinacolone	1.2	1.49	-0.29
Pindolol	1.92	1.6	0.32
Pipamperone	2.02	1.87	0.15
Piperazine	-1.17	-1.03	-0.14
Piperidine	0.85	0.75	0.10
Piperonal	1.05	1.5	-0.45
Piperonyl alcohol	1.05	1.17	-0.12
Pipracil	0.5	-0.03	0.53
Piracetam	-1.54	-1.13	-0.41
Pirenzepine	0.6	0.45	0.15
Piretanide	1.5	1.74	-0.24

Pirimicarb	1.7	1.68	0.02
Piroxicam	3.06	3.41	-0.35
p-Isopropylphenyl diphenyl phosphate	5.7	5.22	0.48
Pivalone	3	2.57	0.43
Pivalonitrile	1.08	1.38	-0.30
p-Menthadiene	4.38	4.07	0.31
Practolol	0.79	0.95	-0.16
Prazepam	3.72	3.91	-0.19
Prednisolone	1.62	1.65	-0.03
Prednisone	1.47	1.67	-0.20
Preforan	3.65	4.53	-0.88
Pregnenolone	4.22	4.6	-0.38
Prehnitene	3.98	3.79	0.19
Proazamine	4.81	4.45	0.36
Probarbital	0.97	0.72	0.25
Procainamide	0.88	0.96	-0.08
Procaine	1.92	1.8	0.12
Procarbazine	0.06	0.23	-0.17
Procodazole	1.3	1.59	-0.29
Procymidone	3	2.94	0.06
Progabide	2.97	3.12	-0.15
Progesterone	3.87	4.74	-0.87
Promazine	4.55	4.46	0.09
Promecarb	3.1	2.85	0.25
Prometon	2.99	3.29	-0.30
Prometryn	3.51	3.59	-0.08
Pronamide	3.26	2.92	0.34
Propachlor	2.18	2.41	-0.23
Propanal	0.59	0.71	-0.12
Propandioic acid	-0.81	-0.17	-0.64
Propane	2.36	1.98	0.38
Propanenitrile	0.16	0.74	-0.58
Propanil	3.07	2.98	0.09
Propanoic acid	0.33	0.59	-0.26
Propanoic anhydride	0.4	1.38	-0.98
Propanolamine	-1.12	-1.04	-0.08
Propanone	-0.24	0.41	-0.65
Propargyl acetate	0.28	0.57	-0.29
Propargyl propionate	0.81	1.01	-0.20
Propargylamine	-0.43	-0.49	0.06
Propazine	2.93	3.04	-0.11
Propenal	-0.01	0.49	-0.50

Propham	2.6	2.61	-0.01
Propiolic acid	-0.52	-0.19	-0.33
Propionanilide	1.61	1.92	-0.31
Propoxur	1.52	2.28	-0.76
Propranolol	2.98	2.7	0.28
Propyl 4-hydroxybenzoate	3.04	2.25	0.79
Propyl butyrate	2.3	2.23	0.07
Propyl chloroformate	1.12	1.08	0.04
Propyl isothiocyanate	2.42	2.67	-0.25
Propyl N-methylcarbamate	0.95	0.62	0.33
Propyl propanoate	1.77	1.79	-0.02
Propyl valerate	2.83	2.67	0.16
Propyl-1,2-dinitrate	1.83	2.32	-0.49
Propylene	1.77	1.55	0.22
Propylenecarbonate	-0.41	0.32	-0.73
Propylisopropylacetamide	1.48	1.83	-0.35
Propyne	0.94	0.99	-0.05
Prostaglandin F2A	2.28	3.21	-0.93
Prosulfuron	2.8	3.13	-0.33
Proxyphylline	-0.77	-0.6	-0.17
Prozac	3.82	4.72	-0.90
Pseudococaine	2.09	2.4	-0.31
p-Terphenyl	6.03	5.87	0.16
p-Toluidine	1.39	1.66	-0.27
p-Tolyl N,N-dimethylcarbamate	2.03	2.13	-0.10
Pulegone	3.08	2.79	0.29
Purine	-0.37	-0.28	-0.09
Pyrazinamide	-1.88	-2.1	0.22
Pyrazine	-0.22	-0.47	0.25
Pyrazon	1.14	0.27	0.87
Pyrene	5.08	5.05	0.03
Pyridine	0.65	0.88	-0.23
Pyrimidine	-0.4	-0.15	-0.25
Pyrrole	0.75	0.58	0.17
Pyrrolidine	0.46	0.45	0.01
Quadricyclane	2.9	3.1	-0.20
Quatrimycin	-1.47	-1.73	0.26
Quazepam	4.03	4.21	-0.18
Quercitrin	0.8	0.39	0.41
Quinazolin-2,4-dione	0.2	0.88	-0.68
Quinazolin-4-one	0.77	0.5	0.27
Quinclorac	3.6	3.07	0.53

Quinine	3.5	2.82	0.68
Quinmerac	0.78	0.95	-0.17
Quinoclamine	2.12	1.17	0.95
Quinoline	2.03	2.28	-0.25
Quinoline-1-oxide	0.36	0.89	-0.53
Quinoxaline	1.32	1.33	-0.01
Ranitidine	1.28	1.45	-0.17
Rebemide	1.25	2.26	-1.01
Reglone	-4.6	-4.53	-0.07
Remoxipride	2.13	2.96	-0.83
Renriduron	1.3	1.17	0.13
Retinol	5.68	5.42	0.26
Ribavirin	-2.6	-3.38	0.78
Rivastigmine	2.1	2.51	-0.41
Ronidazole	-0.38	-0.48	0.10
Ropivacaine	2.9	3.47	-0.57
Rosamicin	2.19	1.43	0.76
Saccharin	0.91	0.41	0.50
Saccharose	-3.7	-3.44	-0.26
Salicylanilide	3.27	2.89	0.38
Salicylic acid	2.19	1.56	0.63
Sarin	0.3	0.42	-0.12
s-Butylacrylate	1.78	2.04	-0.26
s-Butylbenzene	4.44	3.93	0.51
s-Butylpropylamine	1.91	2.12	-0.21
Scopolamine	1.24	1.4	-0.16
Secnidazole	0.22	0.56	-0.34
Seconal	2.39	1.82	0.57
Semustine	3.3	2.84	0.46
Serotonin	0.53	1.16	-0.63
Sethoxydim	4.38	4.3	0.08
Simazine	2.18	2.18	0.00
Simvastatin	4.68	5.72	-1.04
Skatole	2.6	2.54	0.06
Soman	1.82	1.5	0.32
Sorbitol	-3.1	-3.53	0.43
s-Phenethyl alcohol	1.42	1.71	-0.29
Stavudine	-0.81	-0.06	-0.75
s-trans-1,3-Butadiene	1.99	1.79	0.20
Stugeron	5.77	5.7	0.07
Styrene	2.95	2.95	0.00
Styrene oxide	1.61	1.94	-0.33

Succinonitrile	-0.99	0.21	-1.20
Sufentanil	3.95	4.11	-0.16
Sulcatone	1.82	2.18	-0.36
Sulfadimidine	0.27	0.86	-0.59
Sulfafurazole	1.01	0.67	0.34
Sulfaguanidine	-1.22	-1.14	-0.08
Sulfamerazine	0.14	0.48	-0.34
Sulfamethoxydiazine	0.41	0.03	0.38
Sulfaperine	0.34	0.44	-0.10
Sulfaphenazole	1.52	1.43	0.09
Sulfasomidine	-0.3	-0.03	-0.27
Sulfathiazole	0.05	0.56	-0.51
Sulfinpyrazone	2.3	1.91	0.39
Sulfolane	-0.77	0.03	-0.80
Sulfometuron-methyl	1.4	0.92	0.48
Sulforidazine	4.45	4.37	0.08
Sulindac	3.6	3.56	0.04
Sulphadiazine	-0.08	0.1	-0.18
Tacrine	3.32	2.89	0.43
Tamoxifen	7.1	6.67	0.43
Tavron	4.56	4.97	-0.41
t-Butyl propionate	1.95	2.03	-0.08
t-Butylamine	0.4	0.68	-0.28
t-Butylbenzene	4.11	3.85	0.26
t-Butylformate	0.97	1.05	-0.08
t-Butylmercaptan	2.14	2.09	0.05
Temaflouxacin	-0.2	-0.04	-0.16
Temazepam	2.19	2.49	-0.30
Terbacil	1.89	2.28	-0.39
Terbufos	4.48	4.59	-0.11
Terbutryne	3.74	3.56	0.18
Terfenadine	7.1	6.94	0.16
Testosterone	3.32	4.02	-0.70
Tetrabromo-2-trifluoromethylbenzimidazole	4.81	5.02	-0.21
Tetracene	5.9	5.59	0.31
Tetrachloro-2-trifluoromethylbenzimidazole	3.97	4.54	-0.57
Tetrachlorocatechol	4.29	3.55	0.74
Tetrachloroethylene	3.4	3.15	0.25
Tetrachloroveratrole	4.86	4.21	0.65
Tetracosane	12.53	13.11	-0.58
Tetradecane	8	7.81	0.19
Tetrahydrofuran	0.46	0.77	-0.31

Tetrahydropyran	0.95	1.07	-0.12
Tetramethylene glycol	0.27	-0.25	0.52
Tetramethylguanidine	0.41	-0.05	0.46
Tetramethylurea	0.19	-0.1	0.29
Tetraphenylmethane	7.88	8.05	-0.17
Tetrazepam	2.76	3.11	-0.35
Tetroxoprim	0.56	1.32	-0.76
Theophylline	-0.18	-0.18	0.00
Thiamazole	-0.34	-0.35	0.01
Thiameturon	0.02	0.57	-0.55
Thiamphenicol	-0.27	-0.48	0.21
Thianaphthene	3.12	3.37	-0.25
Thianthrene	4.57	5.01	-0.44
Thiazole	0.44	0.42	0.02
Thiazone	1.4	1.42	-0.02
Thimet	3.56	3.82	-0.26
Thioacetamide	-0.26	-0.41	0.15
Thioacetanilide	1.71	1.81	-0.10
Thioacetic acid	0.14	0.15	-0.01
Thioanisole	2.74	2.7	0.04
Thiobencarb	3.4	4.18	-0.78
Thiolane	1.61	1.64	-0.03
Thiolane 1-oxide	-0.96	-0.6	-0.36
Thiophanate-ethyl	1.4	1.33	0.07
Thiophene	1.81	2.23	-0.42
Thiophos	3.83	3.85	-0.02
Thioridazine	5.9	5.85	0.05
Thiourea	-1.02	-1.26	0.24
Thioxamyl	-0.47	-0.4	-0.07
Thioxanthone	3.99	3.65	0.34
Threonine	-3.5	-3.78	0.28
Thyreoliberin	-2.47	-3	0.53
Tiabendazole	1.94	2.09	-0.15
Tiapride	0.9	1.3	-0.40
Tinidazole	0.23	0.26	-0.03
t-Nitrobutane	1.17	1.38	-0.21
TNT	1.73	2.18	-0.45
Tolane	4.78	4.55	0.23
Tolazoline	2.65	1.89	0.76
Tolbutamide	2.34	2.08	0.26
Tolclofos-methyl	4.56	4.52	0.04
Toliprolol	1.93	2.04	-0.11

Tolmetin	2.79	2.79	0.00
t-Pentylcarbamate	0.94	1.04	-0.10
t-Pentylisothiocyanate	3.13	3.5	-0.37
Tralkoxydim	4.46	4.62	-0.16
Tramadol	2.63	2.35	0.28
Tranexamic acid	-1.87	-1.5	-0.37
trans-1,2-Cycloheptyl dinitrate	3.41	3.05	0.36
trans-1,2-Cyclohexyl dinitrate	2.62	2.75	-0.13
trans-1,2-Dichloroethylene	2.09	1.75	0.34
trans-1,3-Cyclohexyl dinitrate	2.89	2.75	0.14
trans-1,3-Dichloropropene	1.41	1.81	-0.40
trans-1-Propenylbenzene	3.35	3.23	0.12
trans-2,5-Dimethyltetrahydrofuran	1.34	1.71	-0.37
trans-2-Butene	2.31	1.83	0.48
trans-2-Hepten-1-ol	1.93	1.74	0.19
trans-2-Hexen-1-ol	1.4	1.3	0.10
trans-2-Methylcyclohexanol	1.84	1.51	0.33
trans-2-Nonenoic acid	3.53	2.83	0.70
trans-2-Octenoic acid	3	2.39	0.61
trans-2-Pentenoic acid	1.41	1.07	0.34
trans-2-Phenylcyclopropylamine	1.49	1.78	-0.29
trans-3-Hexenoic acid	1.4	1.51	-0.11
trans-3-Pentenitrile	0.71	1.22	-0.51
trans-3-Phenyl-2-propen-1-ol	1.95	1.72	0.23
trans-3-Phenyl-2-propenenitrile	1.96	2.08	-0.12
trans-4-Methylcyclohexanol	1.79	1.51	0.28
trans-Cinnamic acid	2.08	1.93	0.15
trans-Stilbene	4.81	4.63	0.18
Trazodone	2.9	3.28	-0.38
Triallate	4.29	4.96	-0.67
Triasulfuron	1.6	2.25	-0.65
Triazamate	1.62	2.07	-0.45
Triazolam	5.5	5.5	0.00
Tribenuron-methyl	1.5	0.76	0.74
Tributyl phosphate	4.01	4.01	0.00
Trichlormethiazide	0.56	0.14	0.42
Trichloroacetamide	1.04	0.59	0.45
Trichloroacetic acid	1.33	1.48	-0.15
Trichloroacetonitrile	2.09	1.63	0.46
Trichloroethylene	2.53	2.45	0.08
Trichloromethylthiobenzene	3.78	3.8	-0.02
Trichlorosyringol	3.74	3.28	0.46

Triclosan	4.76	5.05	-0.29
Tridecane	7.33	7.28	0.05
Triethanolamine	-1	-1.7	0.70
Triethyl phosphate	0.8	1.37	-0.57
Triethylamine	1.45	1.77	-0.32
Triflumethazine	4.36	4.28	0.08
Triflumizole	1.4	2.23	-0.83
Trifluoperazine	5.03	5.06	-0.03
Trifluoroacetamide	0.12	-0.15	0.27
Trifluoroacetanilide	2.21	2.07	0.14
Trifluoroacetic acid	0.5	0.74	-0.24
Trifluoroacetophenone	2.15	2.3	-0.15
Trifluoromethylthiobenzene	3.57	4.08	-0.51
Trifluralin	5.34	4.57	0.77
Triflusulfuron-methyl	3.4	3.27	0.13
Triforine	2.2	1.99	0.21
Trihexyphenidyl	4.49	4.34	0.15
Trimellitic anhydride	0.99	0.82	0.17
Trimeprazine	4.71	4.74	-0.03
Trimethadione	-0.37	-0.03	-0.34
Trimethoprim	0.91	1.46	-0.55
Trimethyl phosphate	-0.52	0.08	-0.60
Trimethylacetic acid	1.47	1.23	0.24
Trimethylamine	0.16	0.12	0.04
Trimethyleneglycol dinitrate	1.68	1.87	-0.19
Trimetrexate	2.55	2.32	0.23
Triphenyl phosphate	3.9	4.16	-0.26
Triphenylamine	5.74	4.9	0.84
Triprolidine	3.92	3.93	-0.01
Tripropyl phosphate	1.87	2.69	-0.82
Tripropylamine	2.79	3.09	-0.30
Triptanol	4.93	5.48	-0.55
Tris(2-chloroethyl) phosphate	1.48	1.55	-0.07
Tris-BP	4.39	4.22	0.17
Tropolone	0.53	0.99	-0.46
Trovaflouxacin	0.15	-0.59	0.74
Tryptophane	-1.04	-1.21	0.17
Tyrosine	-1.8	-1.58	-0.22
Undecane	6.31	6.22	0.09
Undecanedioic acid	2.85	2.84	0.01
Undecanonitrile	4.37	4.26	0.11
Uracil	-1.07	-0.67	-0.40

Urea	-1.66	-1.3	-0.36
Uridine	-1.71	-2.57	0.86
Valeryl chloride	2.46	2.6	-0.14
Valine	-2.1	-2.2	0.10
Valium	2.99	2.72	0.27
Veratrole	2.18	2.09	0.09
Vernolate	3.84	3.67	0.17
Viagra	1.9	1.71	0.19
Vinclozolin	3.1	2.72	0.38
Vinyl acetate	0.73	0.93	-0.20
Vinyl butyrate	1.81	1.81	0.00
Vinylidenechloride	2.13	2.19	-0.06
Vinylpropionate	1.29	1.37	-0.08
Vitamin B3	-0.37	-0.79	0.42
Vitamin B6	-0.5	-0.35	-0.15
Vitamin C	-1.85	-1.67	-0.18
Vitavax	2.14	1.96	0.18
Voltaren	4.51	4.26	0.25
Xylose	-3.02	-2.93	-0.09
Zalcitabine	-1.3	-0.86	-0.44
Zofenopril	3.5	3.25	0.25
Zoocoumarin	3.54	4.15	-0.61