SUPPORTING INFORMATION

Title: Simplified Estimation of the Octanol-Air Partition Coefficient

Authors: Kia Sepassi and Samuel Yalkowsky

Corresponding Author: Kia Sepassi

College of Pharmacy, The University of Arizona

1703 E. Mabel Street

Tucson, AZ 85721

Email: sepassi@pharmacy.arizona.edu

Phone: 520-626-4309

Fax: 520-626-2466

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Appendix I: Chemical Name, CAS Number, Molecular Weight, log of the Experimental Octanol-Air Partition Coefficient, Reference, Boiling Point (Kelvin), Predicted log Octanol-Air Partition Coefficient, log of the Error and Absolute Error in prediction.

Compound	CAS No.	MW	Exper log Koa	Ref	BP (K)	Pred log Koa	Error	AE
Methanol	67-56-1	32.0	2.84	10	338.2	2.84	0.00	0.00
Acetonitrile	75-05-8	41.1	2.31	10	332.8	2.44	-0.13	0.13
Ethanol	64-17-5	46.1	3.20	10	351.5	3.05	0.15	0.15
Acrylnitrile	107-13-1	53.1	2.28	15	350.5	2.74	-0.46	0.46
Propionitrile	107-12-0	55.1	2.69	10	370.3	3.10	-0.41	0.41
Propionitrile	107-12-0	55.1	2.83	15	370.3	3.10	-0.27	0.27
Propanal	123-38-6	58.1	3.02	10	321.2	2.25	0.77	0.77
Acetone	67-64-1	58.1	2.31	10	328.7	2.37	-0.06	0.06

Methyl formate	107-31-3	60.1	1.75	10	304.9	1.99	-0.24	0.24
Acetic Acid	64-19-7	60.1	4.31	10	391.2	3.87	0.44	0.44
2-Propanol	67-63-0	60.1	3.38	10	355.6	3.07	0.31	0.31
1-Propanol	71-23-8	60.1	3.68	10	370.4	3.40	0.28	0.28
Nitromethane	75-52-5	61.0	2.52	10	374.3	3.17	-0.65	0.65
Methyl Acrylonitrile	126-98-7	67.1	2.60	15	363.5	2.97	-0.37	0.37
Butyronitrile	109-74-0	69.1	3.12	10	390.8	3.48	-0.36	0.36
2-Propanenitrile	78-82-0	69.1	2.87	10	377.2	3.22	-0.35	0.35
2-Butanone	78-93-3	72.1	2.85	15	352.7	2.78	0.07	0.07
2-Butanone	78-93-3	72.1	2.77	10	352.7	2.78	-0.01	0.01
Tetrahydrofuran	109-99-9	72.1	2.86	10	338.2	2.53	0.33	0.33
Butanal	123-72-8	72.1	3.39	10	348.0	2.71	0.68	0.68
Dimethylformamide	68-12-2	73.1	4.38	10	426.2	4.17	0.21	0.21
Butylamine	109-73-9	73.1	3.61	10	350.2	2.81	0.80	0.80
Ethyl formate	109-94-4	74.1	2.19	10	327.2	2.35	-0.16	0.16
Methyl acetate	79-20-9	74.1	2.31	10	330.2	2.40	-0.09	0.09
N-Nitrosodimethylamine	62-75-9	74.1	3.72	15	427.2	4.19	-0.46	0.46
Diethyl ether	60-29-7	74.1	2.56	15	307.8	2.04	0.52	0.52
Diethyl ether	60-29-7	74.1	2.19	10	307.8	2.04	0.15	0.15
1-Butanol	71-36-3	74.1	4.19	10	391.2	3.81	0.38	0.38
t-Butanol	75-65-0	74.1	3.50	10	355.6	3.03	0.47	0.47
2-Methyl-1-propanol	78-83-1	74.1	3.93	10	381.2	3.58	0.35	0.35
Nitroethane	79-24-3	75.1	2.88	10	387.2	3.41	-0.53	0.53
Allyl chloride	107-05-1	76.5	1.67	15	318.3	2.20	-0.53	0.53
Benzene	71-43-2	78.1	2.66	15	353.2	2.79	-0.13	0.13
Benzene	71-43-2	78.1	2.80	10	353.2	2.79	0.01	0.01
Dimethyl sulfoxide	67-68-5	78.1	4.96	10	463.2	4.91	0.05	0.05
1-Chloropropane	540-54-5	78.5	2.24	10	319.7	2.23	0.01	0.01
Pyridine	110-86-1	79.1	4.20	15	388.4	3.43	0.77	0.77
gamma-Terpinene	99-85-4	80.1	4.28	16	456.2	4.78	-0.50	0.50
alpha-Terpinene	99-86-5	80.1	3.90	16	448.2	4.61	-0.71	0.71
Pentanonitrile	110-59-8	83.1	3.60	10	414.2	3.95	-0.35	0.35
Cyclopentanone	120-92-3	84.1	3.67	10	403.7	3.72	-0.05	0.05
Dichloromethane	75-09-2	84.9	2.00	15	313.2	2.12	-0.12	0.12
Dichloromethane	75-09-2	84.9	2.27	10	313.2	2.12	0.15	0.15
2-Pentanone	107-87-9	86.1	3.19	10	375.4	3.20	-0.01	0.01
3-Pentanone	96-22-0	86.1	3.20	10	375.1	3.19	0.01	0.01
Tetrahydropyran	142-68-7	86.1	3.22	10	361.2	2.96	0.26	0.26
3-Methyl-2-butanone	563-80-4	86.1	3.04	10	367.5	3.05	-0.01	0.01
Dimethylacetamide	127-19-5	87.1	5.33	10	438.2	4.41	0.92	0.92
1,4-Dioxane	123-91-1	88.1	3.23	15	374.7	3.18	0.05	0.05
1,4-Dioxane	123-91-1	88.1	3.17	10	374.7	3.18	-0.01	0.01
Propyl formate	110-74-7	88.1	2.66	10	354.1	2.82	-0.16	0.16
N-Nitroso-methyl-ethylamine	10595-95-6	88.1	3.85	15	443.2	4.53	-0.68	0.68
Ethyl acetate	141-78-6	88.1	2.70	10	350.3	2.75	-0.05	0.05
Isopentanol	123-51-3	88.1	4.52	10	404.2	4.05	0.47	0.47
Methyl Tertiary Butyl Ether	1634-04-4	88.1	2.58	10	328.4	2.37	0.21	0.21
1-Pentanol	71-41-0	88.2	4.69	10	411.2	4.22	0.47	0.47
1-Nitropropane	108-03-2	89.1	3.25	10	404.2	3.74	-0.49	0.49
Toluene	108-88-3	92.1	3.32	15	383.8	3.34	-0.02	0.02

Toluene	108-88-3	92.1	3.31	10	383.8	3.34	-0.03	0.03
2-Picoline	109-06-8	93.1	4.30	15	402.2	3.69	0.61	0.61
Aniline	62-53-3	93.1	4.48	15	457.2	4.93	-0.45	0.45
Fluorobenzene	462-06-6	96.1	2.84	15	357.9	2.87	-0.03	0.03
cis-1,2-Dichloroethene	156-59-2	96.9	2.32	15	328.2	2.36	-0.04	0.04
1,1-Dichloroethene	75-35-4	96.9	2.34	15	304.9	1.99	0.35	0.35
trans-1,2-Dichloroethene	156-60-5	96.9	1.95	15	320.7	2.24	-0.29	0.29
Hexanonitrile	628-73-9	97.2	4.08	10	436.8	4.42	-0.34	0.34
1,2-Dichloroethane	107-06-2	99.0	2.78	10	356.2	2.85	-0.07	0.07
1,2-Dichloroethane	107-06-2	99.0	2.91	15	356.2	2.85	0.06	0.06
1,1-Dichloroethane	75-34-3	99.0	2.26	15	330.6	2.40	-0.15	0.15
Methyl methacrylate	80-62-6	100.1	3.08	15	373.2	3.16	-0.08	0.08
Cyclohexanol	108-93-0	100.2	5.18	10	434.0	4.65	0.53	0.53
2-Hexanone	591-78-6	100.2	3.68	10	400.2	3.68	0.00	0.00
Hexanal	66-25-1	100.2	4.41	10	404.2	3.77	0.64	0.64
4-Methyl-2-pentanone	108-10-1	100.2	3.30	15	389.7	3.47	-0.17	0.17
2-Hexanone	591-78-6	100.2	3.36	15	400.2	3.68	-0.32	0.32
Dipropyalmine	142-84-7	101.2	3.59	10	383.2	3.43	0.16	0.16
Ethyl Propionate	105-37-3	102.1	3.15	10	372.3	3.15	0.00	0.00
Isopropyl acetate	108-21-4	102.1	2.93	10	361.8	2.95	-0.02	0.02
Propyl acetate	109-60-4	102.1	3.17	10	374.7	3.19	-0.02	0.02
N-nitrosodiethylamine	55-18-5	102.1	4.04	15	450.2	4.69	-0.65	0.65
Di-isopropyl ether	108-20-3	102.2	2.66	10	341.7	2.60	0.06	0.06
Dipropyl ether	111-43-3	102.2	2.97	10	363.2	2.99	-0.02	0.02
1-Hexanol	111-27-3	102.2	5.18	10	431.2	4.64	0.54	0.54
Styrene	100-42-5	104.2	3.93	15	418.2	4.00	-0.07	0.07
Ethyl benzene	100-41-7	106.2	3.70	15	409.4	3.84	-0.14	0.14
p-Xylene	106-42-3	106.2	3.65	15	411.5	3.87	-0.22	0.22
m-Xylene	108-38-3	106.2	3.65	15	412.3	3.89	-0.24	0.24
o-Xylene	95-47-6	106.2	3.91	15	411.7	3.88	0.03	0.03
1-Chlorobutane	109-69-3	106.6	2.72	10	351.2	2.76	-0.04	0.04
o-Toluidine	95-53-4	107.2	4.66	15	473.4	5.26	-0.60	0.60
Anisole	100-66-3	108.1	4.01	10	426.9	4.18	-0.17	0.17
cis-1,3-Dichloropropene	10061-01-5	111.0	3.75	15	385.2	3.38	0.37	0.37
trans-1,3-Dichloropropene	10061-02-6	111.0	3.28	15	385.2	3.38	-0.10	0.10
1,1-Dichloropropene	563-58-6	111.0	2.51	15	349.7	2.73	-0.22	0.22
Chlorobenzene	108-90-7	112.6	3.76	15	404.9	3.74	0.02	0.02
1,2-Dichloropropane	78-87-5	113.0	2.96	10	368.7	3.07	-0.11	0.11
1,2-Dichloropropane	78-87-5	113.0	4.15	15	368.7	3.07	1.08	1.08
1,3-Dichloropropane	142-28-9	113.0	3.53	15	393.6	3.55	-0.02	0.02
2,2-Dichloropropane	594-20-7	113.0	2.30	15	342.2	2.60	-0.30	0.30
1,4-Difluorobenzene	540-36-3	114.1	2.93	15	362.2	2.95	-0.02	0.02
Ethyl Methacrylate	97-63-2	114.1	3.34	15	390.2	3.48	-0.14	0.14
2-Heptanone	110-43-0	114.2	4.15	10	424.2	4.17	-0.02	0.02
Ethyl butanoate	105-54-4	116.2	3.56	10	394.7	3.58	-0.02	0.02
Isobutyl acetate	110-19-0	116.2	3.45	10	389.7	3.48	-0.03	0.03
Butyl acetate	123-86-4	116.2	3.65	10	399.2	3.67	-0.02	0.02
Trichloromethane	67-66-3	119.4	2.80	10	335.2	2.48	0.32	0.32
Trichloromethane	67-66-3	119.4	2.76	15	335.2	2.48	0.28	0.28
Propylbenzene	103-65-1	120.2	4.04	15	432.2	4.30	-0.26	0.26

1,3,5-trimethylbenzene	108-67-8	120.2	4.18	15	437.9	4.40	-0.22	0.22
1,2,4-trimethylbenzene	95-63-6	120.2	4.20	15	442.2	4.48	-0.28	0.28
Isopropylbenzene	98-82-8	120.2	3.96	15	424.2	4.13	-0.17	0.17
trans-1,4-Dichloro-2-butene	110-57-6	125.0	4.15	15	425.7	4.18	-0.03	0.03
cis-1,4-Dichloro-2-butene	1476-11-5	125.0	4.04	15	425.2	4.17	-0.13	0.13
4-Chlorotoluene	106-43-4	126.6	4.15	15	435.2	4.34	-0.19	0.19
2-Chlorotoluene	95-49-8	126.6	4.11	15	432.2	4.28	-0.17	0.17
Naphthalene	91-20-3	128.2	4.61	15	491.1	5.50	-0.89	0.89
Octanal	124-13-0	128.2	5.36	10	444.2	4.61	0.75	0.75
Bromochloromethane	74-97-5	129.4	2.67	15	341.0	2.58	0.09	0.09
Isopentyl acetate	123-92-2	130.2	3.94	10	415.2	3.99	-0.05	0.05
Pentyl acetate	628-63-7	130.2	4.12	10	422.4	4.14	-0.02	0.02
N-nitrosodipropylamine	621-64-7	130.2	4.30	15	479.2	5.34	-1.04	1.04
Dibutyl ether	142-96-1	130.2	3.89	10	413.4	3.98	-0.09	0.09
Di-isobutyl ether	628-55-7	130.2	3.40	10	396.2	3.62	-0.22	0.22
Trichloroethene	79-01-6	131.4	3.41	15	360.4	2.92	0.49	0.49
1,1,2-Trichloroethane	79-00-5	133.4	3.54	15	387.0	3.41	0.13	0.13
1,1,1-Trichloroethane	71-55-6	133.4	2.70	10	347.2	2.69	0.01	0.01
1,1,1-Trichloroethane	71-55-6	133.4	2.62	15	347.2	2.69	-0.07	0.07
Butylbenzene	104-51-8	134.2	4.34	15	456.2	4.81	-0.47	0.47
sec-Butylbenzene	135-98-8	134.2	4.20	15	446.2	4.59	-0.38	0.38
tert-Butylbenzene	98-06-6	134.2	4.18	15	442.2	4.48	-0.31	0.31
p-Isopropyltoluene	99-87-6	134.2	4.54	15	449.7	4.63	-0.09	0.09
beta-Pinene	127-91-3	136.2	3.68	16	439.2	4.42	-0.74	0.74
3-Carene	13466-78-9	136.2	3.80	16	443.2	4.50	-0.70	0.70
Tricyclene	508-32-7	136.2	3.87	16	425.7	4.15	-0.28	0.28
Camphene	79-92-5	136.2	4.04	16	432.2	4.28	-0.24	0.24
alpha-Pinene	80-56-8	136.2	3.75	16	428.2	4.20	-0.45	0.45
Limonene	138-86-3	136.2	4.04	16	451.2	4.67	-0.62	0.62
Iodomethane	74-88-4	141.9	1.46	15	315.7	2.16	-0.70	0.70
2-Methylnaphthalene	91-57-6	142.2	5.11	15	514.2	6.00	-0.88	0.88
Hexyl acetate	142-92-7	144.2	4.58	10	444.7	4.62	-0.04	0.04
1,4-Dichlorobenzene	106-46-7	147.0	4.30	15	446.2	4.56	-0.26	0.26
1,3-Dichlorobenzene	541-73-1	147.0	4.30	15	446.2	4.56	-0.26	0.26
1,2-Dichlorobenzene	95-50-1	147.0	4.32	15	453.2	4.71	-0.39	0.39
1,2,3-Trichloropropane	96-18-4	147.4	4.15	15	430.2	4.24	-0.09	0.09
Acenaphthylene	208-96-8	152.2	6.34	21	538.2	6.52	-0.18	0.18
Tetrachloromethane	56-23-5	153.8	2.79	10	350.2	2.74	0.05	0.05
Tetrachloromethane	56-23-5	153.8	2.76	15	350.2	2.74	0.02	0.02
Acenaphthene	83-32-9	154.2	6.52	21	552.2	6.84	-0.32	0.32
Bromobenzene	108-86-1	157.0	4.08	15	428.2	4.20	-0.12	0.12
N-Nitrosodibutylamine	924-16-3	158.2	4.81	15	507.2	6.01	-1.20	1.20
Dipentyl ether	693-65-2	158.3	4.80	10	461.2	5.02	-0.22	0.22
Dichlorobromomethane	75-27-4	163.8	3.46	15	363.2	2.97	0.49	0.49
Fluorene	86-73-7	166.2	6.90	21	568.2	7.20	-0.30	0.30
Fluorene	86-73-7	166.2	6.59	17	568.2	7.20	-0.61	0.61
1,1,2,2-Tetrachloroethane	79-34-5	167.8	4.36	15	419.7	4.05	0.31	0.31
1,1,1,2-Tetrachloroethane	630-20-6	167.8	3.89	15	403.7	3.73	0.16	0.16
Pentafluorobenzene	363-72-4	168.1	2.54	15	358.2	2.88	-0.33	0.33
Dibromomethane	74-95-3	173.8	3.26	15	370.2	3.09	0.17	0.17

Dibromomethane	74-95-3	173.8	3.07	10	370.2	3.09	-0.02	0.02
4-Bromofluorobenzene	460-00-4	175.0	4.11	15	424.7	4.13	-0.02	0.02
Anthracene	120-12-7	178.2	7.71	21	613.1	8.23	-0.52	0.52
Phenanthrene	85-01-8	178.2	7.68	21	613.2	8.23	-0.55	0.55
Phenanthrene	85-01-8	178.2	7.57	17	613.2	8.23	-0.66	0.66
Teramethyl tin	594-27-4	178.9	2.62	10	351.2	2.76	-0.14	0.14
1,2,4-Trichlorobenzene	120-82-1	181.5	4.59	15	486.7	5.41	-0.82	0.82
1,2,3-Trichlorobenzene	87-61-6	181.5	4.66	15	491.7	5.51	-0.85	0.85
Hexafluorobenzene	392-56-3	186.1	2.11	15	353.4	2.79	-0.68	0.68
1,2-Dibromoethane	106-93-4	187.9	3.69	15	404.8	3.75	-0.06	0.06
PCB-3	2051-62-9	188.7	6.80	20	564.2	7.11	-0.31	0.31
1,4-Dichloronapthalene	1825-31-6	197.1	6.78	20	561.2	7.04	-0.26	0.26
1,2-Dichloronapthalene	2050-69-3	197.1	6.89	20	569.7	7.23	-0.34	0.34
Pentachloroethane	76-01-7	202.3	4.38	15	433.0	4.31	0.07	0.07
Fluoranthene	206-44-0	202.3	8.76	21	648.2	9.05	-0.29	0.29
Pyrene	129-00-0	202.3	8.80	17	677.2	9.74	-0.94	0.94
Fluoranthene	206-44-0	202.3	8.88	17	648.2	9.05	-0.17	0.17
Dibromochloromethane	124-48-1	208.3	3.97	15	393.2	3.52	0.45	0.45
1-Chlorodibenzo-p-dioxin	39227-53-7	218.6	7.86	18	589.2	7.68	0.18	0.18
PCB-15	2050-68-2	223.1	7.73	20	590.2	7.70	0.03	0.03
Chrysene	218-01-9	228.3	10.30	21	721.2	10.81	-0.51	0.51
Benzo[a]anthracene	56-55-3	228.3	10.28	21	710.8	10.55	-0.27	0.27
1,2-Dibromo-3-Chloropropane	96-12-8	236.3	4.56	15	469.2	5.08	-0.52	0.52
Tetrachloroethene	127-18-4	236.7	3.79	15	394.5	3.55	0.24	0.24
Tetrachloroethene	127-18-4	236.7	3.48	10	394.5	3.55	-0.07	0.07
Benzo[k]fluoranthene	207-08-9	252.3	11.37	21	753.2	11.59	-0.22	0.22
Benzo[a]pyrene	50-32-8	252.3	11.56	21	768.2	11.96	-0.40	0.40
Bromoform	75-25-2	252.7	4.23	15	423.2	4.10	0.13	0.13
2,7-Dichlorodibenzo-p-dioxin	33857-26-0	253.1	8.36	18	647.2	9.03	-0.67	0.67
2,8-Dichlorodibenzo-p-dioxin	38964-22-6	253.1	8.36	18	656.2	9.24	-0.88	0.88
Hexachlorobutadiene	87-68-3	260.8	4.58	15	488.2	5.45	-0.87	0.87
1,4,6,7-Tetrachloronapthalene	55720-43-9	266.0	8.13	20	604.2	8.02	0.11	0.11
Indeno[1,2,3-cd]pyrene	193-39-5	276.3	12.43	21	809.2	12.99	-0.56	0.56
Dibenz[a,h]anthracene	53-70-3	278.4	12.59	21	808.2	12.96	-0.37	0.37
Hexachlorobenzene	118-74-1	284.8	7.38	19	598.2	7.88	-0.50	0.50
alpha-Hexachlorocyclohexane	319-84-6	290.8	7.61	19	561.2	7.04	0.57	0.57
gamma-Hexachlorocyclohexane	58-89-9	290.8	7.85	19	596.2	7.84	0.01	0.01
2,3,7,8-Tetrachlorodibenzofuran	51207-31-9	306.0	10.02	18	711.5	10.57	-0.55	0.55
p,p'-DDE	72-55-9	318.0	9.68	19	609.2	8.18	1.50	1.50
p,p'-DDD	72-54-8	320.1	10.10	19	623.2	8.55	1.55	1.55
2,3,7,8-tetrachlorodibenzo-p-dioxin	1746-01-6	322.0	10.05	18	720.2	10.78	-0.73	0.73
1,2,3,4-tetrachlorodibenzo-p-dioxin	30746-58-8	322.0	9.70	18	692.2	10.10	-0.40	0.40
Decafluorobiphenyl	434-90-2	334.1	4.54	15	479.2	5.25	-0.70	0.70
1,2,3,4,7,-Pentachlorodibenzo-p-dioxin	39227-61-7	356.4	10.67	18	738.2	11.22	-0.55	0.55
Heptachlor	76-44-8	373.3	7.64	19	583.2	7.54	0.10	0.10
Dieldrin	60-57-1	380.9	8.90	19	603.2	8.00	0.90	0.90
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	39227-28-6	390.9	11.11	18	761.2	11.79	-0.68	0.68

Oxychlordane	27304-13-8	423.8	8.39	19	626.2	8.53	-0.14	0.14
1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	35822-46-9	425.3	11.42	18	780.4	12.27	-0.85	0.85

Appendix II: Chemical Name, CAS Number, Molecular Weight, log of the Experimental Octanol-Air Partition Coefficient, Reference, Boiling Point (Kelvin), Predicted log Octanol-Air Partition Coefficient, log of the Error and Absolute Error in prediction.

Compound	CAS No.	MW	Exper log Koa	Ref	BP (K)	Pred log Koa	Error	AE
2-Methylbuta-1,3-diene	78-79-5	68.1	2.06	10	307.2	2.03	0.03	0.03
Pyrrolidine	123-75-1	71.1	4.07	10	359.7	2.98	1.09	1.09
Pentane	109-66-0	72.2	1.95	10	309.3	2.06	-0.11	0.11
2-Butanol	78-92-2	74.1	3.80	10	372.7	3.40	0.40	0.40
Carbon disulphide	75-15-0	76.1	2.28	10	319.2	2.22	0.06	0.06
2-Chloroethanol	107-07-3	80.5	4.30	10	402.2	4.02	0.28	0.28
Cyclohexane	110-82-7	84.2	2.71	10	353.9	2.80	-0.09	0.09
1-Hexene	592-41-6	84.2	2.41	10	336.2	2.51	-0.10	0.10
N-methylpyrrolidine	120-94-5	85.1	3.64	10	354.2	2.81	0.83	0.83
Piperidine	110-89-4	85.2	4.04	10	379.5	3.34	0.70	0.70
cis-1,2-Dichloroethene	156-59-2	96.9	2.56	10	328.2	2.36	0.20	0.20
1,1-Dichloroethane	75-34-3	99.0	2.41	10	330.6	2.40	0.01	0.01
Benzonitrile	100-47-0	103.1	4.46	10	464.2	4.93	-0.47	0.47
Ethyl benzene	100-41-4	106.2	3.72	10	409.4	3.84	-0.12	0.12
m-Xylene	108-38-3	106.2	3.79	10	412.3	3.89	-0.10	0.10
o-Xylene	95-47-6	106.2	3.90	10	411.7	3.88	0.02	0.02
Bromoethane	74-96-4	109.0	2.11	10	311.7	2.10	0.01	0.01
1-Octene	111-66-0	112.2	3.35	10	394.2	3.58	-0.23	0.23
Octane	111-65-9	114.2	3.30	10	398.8	3.68	-0.38	0.38
Propylbenzene	103-65-1	120.2	4.09	10	432.2	4.30	-0.21	0.21
Isopropylbenzene	98-82-8	120.2	3.98	10	424.2	4.13	-0.15	0.15
1-Nonene	124-11-8	126.2	3.83	10	420.1	4.11	-0.28	0.28
Naphthalene	91-20-3	128.2	5.19	10	491.1	5.50	-0.31	0.31
1-Octanol	111-87-5	128.2	6.03	10	468.2	5.45	0.58	0.58
Trichloroethene	79-01-6	131.4	2.99	10	360.4	2.92	0.07	0.07
1,1,2-Trichloroethane	79-00-5	133.4	3.40	10	387.0	3.41	-0.01	0.01
Iodomethane	74-88-4	141.9	2.16	10	315.7	2.16	0.00	0.00
1,4-Dichlorobenzene	106-46-7	147.0	4.46	10	446.2	4.56	-0.10	0.10
1,2-Dichlorobenzene	95-50-1	147.0	4.36	10	453.2	4.71	-0.35	0.35
Acenaphthene	83-32-9	154.2	6.31	10	552.2	6.84	-0.53	0.53
Biphenyl	92-52-4	154.2	6.15	10	529.2	6.33	-0.18	0.18
Iodoethane	75-03-6	156.0	2.59	10	345.2	2.65	-0.06	0.06
Hexamethylbenzene	87-85-4	162.3	6.31	10	536.6	6.49	-0.18	0.18
Fluorene	86-73-7	166.2	6.83	10	568.2	7.20	-0.37	0.37
Diphenylamine	122-39-4	169.2	7.64	10	575.2	7.53	0.11	0.11
Anthracene	120-12-7	178.2	7.55	10	613.1	8.23	-0.68	0.68
Phenanthrene	85-01-8	178.2	7.52	10	613.2	8.23	-0.71	0.71
t-Stilbene	103-30-0	180.2	7.48	10	579.7	7.50	-0.02	0.02
1,3,5-Trichlorobenzene	108-70-3	181.5	4.85	10	481.2	5.29	-0.44	0.44
1,2,3-Trichlorobenzene	87-61-6	181.5	5.19	10	491.7	5.51	-0.32	0.32
Pyrene	129-00-0	202.3	8.75	10	677.2	9.74	-0.99	0.99
Fluoranthene	206-44-0	202.3	8.61	10	648.2	9.05	-0.44	0.44
Dibromochloromethane	124-48-1	208.3	3.59	10	393.2	3.52	0.07	0.07

1,2,3,5-Tetrachlorobenzene	634-90-2	215.9	5.55	10	519.2	6.11	-0.56	0.56
1,2,4,5-Tetrachlorobenzene	95-94-3	215.9	5.62	10	517.7	6.07	-0.45	0.45
1,2,3,4-Tetrachlorobenzene	634-66-2	215.9	5.64	10	527.2	6.28	-0.64	0.64
1,4-Dibromobenzene	106-37-6	235.9	5.21	10	492.2	5.52	-0.31	0.31
Hexachloroethane	67-72-1	236.7	4.47	10	462.2	4.89	-0.42	0.42
1-Hexadecanol	36653-82-4	242.5	9.90	10	607.2	9.00	0.90	0.90
Pentachlorobenzene	608-93-5	250.3	6.49	10	550.2	6.79	-0.30	0.30
Hexachlorobenzene	118-74-1	284.8	7.17	10	598.2	7.88	-0.71	0.71
1-Eicosanol	629-96-9	298.6	12.06	10	645.2	10.15	1.91	1.91