

Supplementary Information for “Oligomeric models for estimation of polydimethylsiloxane-water partition ratios with COSMO-RS theory: Impact of the combinatorial term on absolute error” by J. Mark Parnis and Donald Mackay.

Contents:

1) The complete set of chemicals, with the published values of $\log K(\text{PDMS-w})$, and the abbreviated reference, corresponding to references given in the principle text.

1) The complete set of chemicals, with the published values of log K_{PDMS-w} .

Kwon and Meyer 2007 Shake method		1,2,3-trichlorobenzene	3.42
terbutryn	2.66	1,2,4-trichlorobenzene	3.46
diuron	1.10	1,3,5-trichlorobenzene	3.61
carbofuran	0.77	naphthalene	2.85
carbaryl	1.09	acenaphthene	3.46
aldicarb	0.35	KWON and MEYER 2007 ABL Perm	
aniline	0.01	1,2,3-trichlorobenzene	3.46
2-chloroaniline	1.04	1,2,4-trichlorobenzene	3.51
3-chloroaniline	0.83	1,3,5-trichlorobenzene	3.67
3,4-dimethylaniline	1.07	2,4,5-trichlorotoluene	4.21
2,4-dichloroaniline	1.69	1,2,3,5-tetrachlorobenzene	4.12
3,4-dichloroaniline	1.39	1,2,4,5-tetrachlorobenzene	4.03
2,3,5,6-tetrachloroaniline	3.25	pentachlorobenzene	4.56
phenol	-0.53	hexachlorobenzene	4.91
2-chlorophenol	0.56	phenanthrene	3.87
4,6-dinitro-o-toluene	1.23	anthracene	3.98
2,4,6-trichlorophenol	1.73	fluoranthene	4.32
pentachlorophenol	2.65	pyrene	4.36
1,2-dichlorobenzene	2.92	chrysene	4.74
1,4-dichlorobenzene	2.91	benz[a]anthracene	4.85
1,2,3-trichlorobenzene	3.33	benzo[a]pyrene	5.09
1,2,4-trichlorobenzene	3.33	perylene	4.98
1,3,5-trichlorobenzene	3.36	dibenz[a,c]anthracene	5.41
naphthalene	2.75	dibenz[a,h]anthracene	5.47
acenaphthene	3.46	KWON and MEYER 2007 Lit. avg.	
Kwon and Meyer 2007 PCDM method		benzo[ghi]perylene	5.36
2,4,5-trichlorotoluene	4.12	pentachlorobenzene	4.10
1,2,3,5-tetrachlorobenzene	4.24	hexachlorobenzene	4.54
1,2,4,5-tetrachlorobenzene	4.14	naphthalene	3.00
pentachlorobenzene	4.69	acenaphthene	3.63
hexachlorobenzene	5.12	phenanthrene	3.70
phenanthrene	3.74	anthracene	3.75
anthracene	3.93	fluoranthene	4.22
fluoranthene	4.21	pyrene	4.33
pyrene	4.27	chrysene	4.83
chrysene	4.81	benz[a]anthracene	4.55
benz[a]anthracene	4.90	benzo[a]pyrene	4.81
benzo[a]pyrene	5.36	dibenz[a,h]anthracene	4.86
1,2-dichlorobenzene	2.81	benzo[ghi]perylene	4.84
1,4-dichlorobenzene	2.95		

Hsieh 2011		CHAO 2014	
PCB18	4.91	PCB203	7.09
PCB16	5.12	PCB195	6.89
PCB32	5.12	PCB194	6.79
PCB28,31	5.17	Benzyl alcohol	-0.35
PCB33,53	5.18	4-Fluorophenol	-0.28
PCB22	5.30	m-Cresol	-0.03
PCB52	5.48	Phenethyl alcohol	0.12
PCB47,48	5.49	3-Methylbenzyl alcohol	0.17
PCB44	5.44	3-Chlorophenol	0.31
PCB71	5.49	3,5-Dimethylphenol	0.42
PCB41	5.49	3-Bromophenol	0.46
PCB70	5.79	4-Ethylphenol	0.60
PCB66	5.70	4-Chloroaniline	0.84
PCB95	5.77	Phenyl acetate	0.86
PCB56,60	5.86	Benzonitrile	1.04
PCB101	6.01	Acetophenone	1.04
PCB99	6.17	4-Chloroacetophenone	1.64
PCB83	6.02	Methyl benzoate	1.65
PCB97	6.05	Benzene	1.76
PCB87	6.19	Ethylbenzoate	2.12
PCB85	6.38	Toluene	2.28
PCB110	6.03	4-Chloroanisole	2.37
PCB151	6.31	Chlorobenzene	2.40
PCB135	6.48	Bromobenzene	2.51
PCB149	6.42	o-Xylene	2.69
PCB118	6.23	m-Xylene	2.73
PCB146	6.66	Iodobenzene	2.73
PCB153	6.62	p-Xylene	2.75
PCB105,132	6.40	Ethylbenzene	2.75
PCB179	6.73	Phenol	-0.18
PCB141	6.73	Naphthalene	2.83
PCB138	6.61	Cyclopentane	2.85
PCB163	6.56	4-Chlorotoluene	2.87
PCB158	6.83	Methylcyclopentane	3.13
PCB187	6.96	Propylbenzene	3.14
PCB182	6.96	Isopropylbenzene	3.15
PCB183	6.26	1,3,5-Trimethylbenzene	3.16
PCB128	6.61	1-Methyl-4-Ethylbenzene	3.20
PCB185	6.86	Cyclohexane	3.20
PCB174	7.04	1-Methylnaphthalene	3.26
PCB177	7.02	1,2,4-Trimethylbenzene	3.34
PCB171,202	6.78	tert-Butylbenzene	3.34
PCB180	6.89	Biphenyl	3.37
PCB170	6.82	2,3-Dimethylbutane	3.37
PCB201	7.06	2-Methylpentane	3.51

CHAO 2014		Kang et al. 2016 shake	
3-Methylpentane	3.51	3,3-Dimethyloctane	4.92
1-Methyl-3-Isopropylbenzene	3.52	2,5-Dimethylheptane	4.93
trans-1,2-Dimethylcyclopentane	3.53	3,4-Dimethylheptane	4.97
1-Methyl-3-n-Propylbenzene	3.58	1,4,5-Trimethylnaphthalene	3.74
n-Butylbenzene	3.59	2,4,5-Trimethylnaphthalene	3.72
1,2-Dimethyl-4-Ethylbenzene	3.60	9,9-Dimethylfluorene	3.76
sec-Butylbenzene	3.60	9-Methylanthracene	4.24
Isobutylbenzene	3.62	Kang et al. 2016 ABL perm	
cis-1,3-Dimethylcyclopentane	3.63	1,4,5-Trimethylnaphthalene	3.74
1,3-Dimethyl-2-Ethylbenzene	3.64	2,4,5-Trimethylnaphthalene	3.72
Methylcyclohexane	3.67	9,9-Dimethylfluorene	3.76
1,2,4-Trimethylcyclopentane(1a,2a,4a)	3.75	9-Methylanthracene	5.52
trans-1,2-Dimethylcyclohexane	3.82	3-Methylphenanthrene	4.16
1-Ethyl-1-methylcyclopentane	3.83	3,6-Dimethylphenanthrene	4.64
2,2-Dimethylpentane	3.87	9,10-Dimethylanthracene	4.52
cis-1,2-Dimethylcyclohexane	3.89	Grant 2016	
n-Pentylbenzene	3.91	log K pdms-w	4.53
2,4-Dimethylpentane	3.95	7-Methylbenz[a]anthracene	4.99
2-Methylbutylbenzene	3.96	7,12-Dimethylbenz[a]anthracene	5.32
2,2,3-Trimethylbutane	3.99	123478-HxCDD	6.42
2-Methylhexane	4.01	1234678-HpCDD	6.68
3,3-Dimethylpentane	4.04	OCDD	7.25
3-Methylhexane	4.05	OCDF	7.44
2,3-Dimethylpentane	4.12	PCB182	6.63
1,2,4-Triethylbenzene	4.21	Eganhouse 2016 averaged	
1,3,5-Triethylbenzene	4.27	PCB204	6.88
2,2,3-Trimethylpentane	4.33	PCB206	7.45
2,5-Dimethylhexane	4.37	PCB209	7.59
2,2-Dimethylhexane	4.39	Bis(p-chlorophenyl)ethane	5.55
2-Methylheptane	4.41	DDNU (VAN)	5.84
4-Methylheptane	4.44	DDMU	5.97
3-Ethylhexane	4.45	1-Chloro-2-[2,2-dichloro-1-(4-chlorophenyl)vinyl]benzene	6.35
3-Methylheptane	4.50	1,1'-(2-Chloro-1,1-ethanediyl)bis(4-chlorobenzene)	5.14
2,3-Dimethylhexane	4.53	dichlorodiphenyldichloroethylene	6.37
2,4-Dimethylhexane	4.61	Mitotane	5.44
2-Methyloctane	4.66	Dichlorodiphenyldichloroethane	5.27
3,3-Diethylpentane	4.80	1-Chloro-2-[2,2,2-trichloro-1-(4-chlorophenyl)ethyl]benzene	6.48
3-Methyloctane	4.82	DDT	6.18
2,3-Dimethylheptane	4.84	PCB49	6.08
3,3-Dimethylheptane	4.88	PCB28	5.72
3,5-Dimethylheptane	4.90	PCB52	6.01
		PCB44	5.96
		PCB70	6.12
		PCB66	6.13
		PCB101	6.52
		PCB87	6.51
		PCB110	6.46
		PCB118	6.59
		PCB153	6.98
		PCB138	6.98