Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Table S1. Experimental log K_{srw} values and log K_{ow} values for 119 chemicals in training and validation sets

ID	Cas no.	Name	logK_{ow}	logK_{srw}
1	91-20-3	Naphthalene	3.35 [1]	3.28 [1, 2]
2	208-96-8	Acenaphthylene	3.61 [1]	3.33 [1, 2]
3	83-32-9	Acenaphthene	3.92 [1]	3.73 [1, 2]
4	86-73-7	Fluorene	4.18 [1]	3.84 [1, 2]
5	91-57-6	2-Methylnaphthalene	4 [1]	4.06 [1]
6	90-12-0	1-Methylnaphthalene	3.87 [1]	4 .00[1]
7	85-01-8	Phenanthrene	4.52 [1]	4.07 [1-3]
8	120-12-7	Anthracene	4.5 [1]	4.19 [1-3]
9	2531-84-2	2-Methylphenanthrene	5.24 [1]	4.89 [1]
10	1576-67-6	3,6-Dimethylphenanthrene	5.25 [1]	5.15 [1]
11	66271-32-7	2,6,9-Trimethylphenanthrene	5.99 [1]	5.34 [1]
12	132-65-0	Dibenzothiophene	4.38 [1]	4.04 [1]
13	206-44-0	Fluoranthene	5.2 [1]	4.50 [1-3]
14	129-00-0	Pyrene	5 [1]	4.54 [1-3]
15	25889-60-5	1-Methylfluoranthene	5.48 [1]	5.01 [1]
16	15679-24-0	2,7-Dimethylpyrene	6.03 [1]	6.30 [1]
17	195-19-7	Benzo[*c*]phenanthrene	5.76 [1]	5.38 [1]
18	56-55-3	Benz[*a*]anthracene	5.91 [1]	5.26 [1-3]
19	218-01-9	Chrysene	5.86 [1]	5.14 [1-3]
20	3351-32-4	2-Methylchrysene	6.88 [1]	6.15 [1]
21	205-99-2	Benzo[*b*]fluoranthene	5.78 [1]	5.94 [1, 3]
22	207-08-9	Benzo[*k*]fluoranthene	6.11 [1]	5.91 [1, 3]
23	192-97-2	Benzo[*e*]pyrene	6.44 [1]	5.78 [1, 3]
24	50-32-8	Benzo[*a*]pyrene	6.35 [1]	5.83 [1-3]
25	198-55-0	Perylene	6.25 [1]	6.02 [1]

26	63041-77-0	7-Methylbenzo[*a*]pyrene	6.66 [a]	6.97 [1]
27	193-39-5	Indeno[*1,2,3-cd*]pyrene	7.66 [1]	6.55 [1-3]
28	191-24-2	Benzo[*g,h,i*]perylene	6.9 [1]	6.21 [1-3]
29	53-70-3	Dibenz[*a,h*]anthracene	6.75 [1]	6.39 [1-3]
30	7012-37-5	PCB 28	5.67 [1]	5.2 [1-3]
31	16606-02-3	PCB 31	5.67 [1]	5.08 [1, 2]
32	37680-69-6	PCB 35	5.82 [1]	4.56 [1]
33	41464-39-5	PCB 44	5.75 [1]	5.51 [1, 2]
34	41464-40-8	PCB 49	5.85 [1]	5.55 [1, 2]
35	35693-99-3	PCB 52	5.84 [1]	5.48 [1-3]
36	41464-41-9	PCB53	5.62 [1]	5.02 [1]
37	32598-11-1	PCB 70	6.2 [1]	5.17 [1]
38	32690-93-0	PCB 74	6.2 [1]	5.29 [1]
39	41464-51-1	PCB 97	6.29 [1]	5.85 [1, 2]
40	38380-01-7	PCB 99	6.39 [1]	6.03 [1, 2]
41	37680-73-2	PCB 101	6.38 [1]	6.08 [1-3]
42	32598-14-4	PCB 105	6.65 [1]	6.01 [1, 2]
43	38380-03-9	PCB 110	6.48 [1]	6.02 [1, 2]
44	74472-36-9	PCB 112	6.45 [1]	5.59 [1]
45	31508-00-6	PCB 118	6.74 [1]	6.26 [1-3]
46	38380-07-3	PCB 128	6.74 [1]	6.43 [1, 2]
47	38380-05-1	PCB 132	6.58 [1]	5.79 [1]
48	35694-06-5	PCB 137	6.83 [1]	6.46 [1, 2]
49	35065-28-2	PCB 138	7.88 [3]	6.68 [1-3]
50	38380-04-0	PCB 149	6.67 [1]	6.40 [1, 2]
51	52663-63-5	PCB 151	6.64 [1]	6.33 [1, 2]
52	35065-27-1	PCB 153	7.84 [3]	6.57 [1-3]
53	38380-08-4	PCB 156	7.85 [3]	6.85 [1-3]

54	69782-90-7	PCB 157	7.18 [1]	6.06 [1]
55	74472-42-7	PCB 158	7.02 [1]	6.20 [1]
56	35065-30-6	PCB 170	8.62 [3]	6.96 [1-3]
57	35065-29-3	PCB 180	8.58 [3]	6.92 [1-3]
58	52663-69-1	PCB 183	7.2 [1]	6.67 [1]
59	52663-68-0	PCB 187	8.53 [3]	6.89 [1-3]
60	39635-31-9	PCB 189	7.24 [1]	6.45 [1]
61	2051-24-3	PCB 209	8.18 [1]	7.81 [1]
62	87-68-3	Hexachloro-1,3-butadiene	5.43 [3]	4.68 [3]
63	118-74-1	Hexachlorobenzene	6.2 [3]	4.99 [2, 3]
64	37680-65-2	PCB-18	5.89 [3]	5.15 [2, 3]
65	41464-42-0	PCB-72	6.42 [3]	5.82 [3]
66	60145-21-3	PCB-103	7.16 [3]	6.15 [3]
67	32598-10-0	PCB-66	6.46 [3]	5.88 [2, 3]
68	33979-03-2	PCB-155	7.85 [3]	6.84 [2, 3]
69	32598-13-3	PCB-77	6.44 [3]	5.64 [3]
70	57465-28-8	PCB-126	7.1 [3]	5.98 [3]
71	32774-16-6	PCB-169	7.77 [3]	6.57 [3]
72	81-14-1	Musk ketone	4.3 [4]	3.05 [4]
73	81-15-2	Musk xylene	4.8 [4]	3.31 [4]
74	145-39-1	Musk tibetene	5.9 [4]	4.15 [4]
75	83-66-9	Musk ambrette	5.7 [4]	3.91 [4]
76	1222-05-5	Galaxolide	5.9 [4]	3.97 [4]
77	1506-02-1	Tonalide	5.7 [4]	4.01 [4]
78	13171-00-1	Celestolide	5.9 [4]	3.96 [4]
79	68140-48-7	Traseolide	6.3 [4]	4.36 [4]
80	15323-35-0	Phantolide	5.9 [4]	3.78 [4]
81	33704-61-9	Cashmeran	4.9 [4]	3.46 [4]

82	54464-57-2	OTNE	5.28 [4]	3.63 [4]
83	3380-34-5	Triclosan	4.76 [4]	3.02 [4]
84	4640-01-1	Methyl triclosan	5.22 [4]	3.62 [4]
85	28159-98-0	Irgarol	4.07 [4]	3.6 [4]
86	25154-52-3	Nonylphenol	5.9 [4]	3.49 [4]
87	27193-28-8	Octylphenol	5.5 [4]	3.28 [4]
88	83834-59-7	2-ethylhexyl methoxycinnamate	5.77 [4]	4.77 [4]
89	36861-47-9	4-methylbenzylidene camphor	4.95 [4]	3.39 [4]
90	118-60-5	2-ethylhexyl salicylate	5.77 [4]	4.70 [4]
91	118-56-9	Homosalate	5.82 [4]	4.55 [4]
92	131-57-7	Benzophenone-3	3.64 [4]	3.08 [4]
93	117-99-7	2-hydroxybenzophenone	3.47 [4]	3.04 [4]
94	6197-30-4	Octocrylene	7.53 [4]	4.96 [4]
95	126-71-6	Tris-isobutylphosphate	3.71 [4]	4.68 [4]
96	126-73-8	Tris-n-butylphosphate	4.26 [4]	5.00 [4]
97	1241-94-7	2-ethylhexyldiphenylphosphate	5.73 [4]	5.39 [4]
98	115-86-6	Triphenylphosphate	4.7 [4]	4.94 [4]
99	78-42-2	Tris-2-ethylhexylphosphate	9.49 [4]	5.88 [4]
100	78-30-8	Tris-o-tolylphosphate	6.3 [4]	5.50 [4]
101	563-04-2	Tris-m-tolylphosphate	6.3 [4]	5.77 [4]
102	1330-78-5	Tris-p-tolylphosphate	6.3 [4]	5.85 [4]
103	13029-08-8	PCB 4	4.65 [2]	4.59 [2]
104	33146-45-1	PCB 10	4.84 [2]	4.55 [2]
105	34883-41-5	PCB 14	5.28 [2]	5.14 [2]
106	55702-46-0	PCB 21	5.51 [2]	5.43 [2]
107	15862-07-4	PCB 29	5.6 [2]	5.43 [2]
108	35693-92-6	PCB 30	5.44 [2]	5.24 [2]
109	2437-79-8	PCB 47	5.85 [2]	5.78 [2]

110	62796-65-0	PCB 50	5.63 [2]	5.70 [2]
111	74338-24-2	PCB 55	6.11 [2]	6.00 [2]
112	41464-43-1	PCB 56	6.11 [2]	6.04 [2]
113	70362-49-1	PCB 78	6.35 [2]	6.05 [2]
114	65510-45-4	PCB 85	6.3 [2]	6.24 [2]
115	38380-02-8	PCB 87	6.29 [2]	6.35 [2]
116	56558-16-8	PCB 104	5.81 [2]	6.17 [2]
117	52712-04-6	PCB 141	6.82 [2]	6.70 [2]
118	74472-40-5	PCB 145	6.25 [2]	6.65 [2]
119	74472-52-9	PCB 204	7.3 [2]	7.59 [2]

[a] The logK_{ow} value was calculated using EPIWEB 4.1 free on-line software (copyright: US Environmental Protection Agency)

Reference

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