

Appendix E:

Range of Reported Values of H and log K_{ow} for Individual Gaseous Hazardous Air Pollutants and Mixtures

Table E.1. Range of reported values of H and log K_{ow} for individual hazardous air pollutants at 293-298 K.

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
1	乙醛 Acetaldehyde	75-07-0	6.0 - 60	5.423 - 10.18	-0.53 - 0.52
2	乙酰胺 Acetamide	60-35-5	NA ^c	3.53 x 10 ⁻⁴	-1.58 - (-1.09)
3	乙腈; 氰化甲烷 Acetonitrile	75-05-8	1.9 - 3.5	2.033 - 3.501	-0.54 - 0.06
4	乙酰苯 Acetophenone	98-86-2	0.92 - 1.1	0.784 - 1.084	1.56 - 1.87
5	2-乙酰氨基苄 2-Acetylamino-fluorene	53-96-3	NA	NA	NA
6	丙烯醛 Acrolein	107-02-8	10 - 14	0.446, 12.36	-0.10 - 0.101
7	丙烯酰胺 Acrylamide	79-06-1	NA	1.44 x 10 ⁻⁴	-1.24 - (-0.67)
8	丙烯酸 Acrylic acid	79-10-7	4.2 x 10 ⁻²	0.042	0.31 - 0.43
9	丙烯腈 Acrylonitrile	107-13-1	9.2, 14	8.918 - 11.14	-0.92 - 1.20
10	烯丙基氯 Allyl chloride	107-05-1	1.1 x 10 ³ , 9.2 x 10 ²	NA	NA
11	4-氨基联二苯 4-Aminobiphenyl	92-67-1	NA	NA	NA
12	苯胺 Aniline	62-53-3	NA	12.16, 13778	0.78 - 1.34
13	邻氨基苯甲醚 o-Anisidine	90-04-0	NA	NA	NA
14	苯 Benzene	71-43-2	4.6 x 10 ² - 8.4 x 10 ²	441 - 740	1.56 - 2.69
15	联苯胺 Benzidine	92-87-5	NA	4.60 x 10 ⁻⁷ , 3.93 x 10 ⁻⁶	1.34 - 2.40
16	三氯甲苯 Benzotrichloride	98-07-7	NA	NA	NA
17	氯化苄 Benzyl chloride	100-44-7	63	NA	NA
18	联苯 Biphenyl	92-52-4	28 - 84	11.55 - 124	3.16 - 4.52
19	双氯甲醚 Bis(chloromethyl) ether	542-88-1	NA	21.27	-0.38, 2.40
20	邻苯二甲酸二(2-乙基己基)酯 Bis(2-ethylhexyl)phthalate	117-81-7	NA	0.0041 - 3.14	3.58 - 9.70
21	三溴甲烷 Bromoform	75-25-2	44 - 72	7.66 - 68.3	2.30 - 2.38
22	1,3-二丁烯 1,3-Butadiene	106-99-0	6.3 x 10 ³ - 7.2 x 10 ³	6227 - 10820	1.56 - 1.99
23	己内酰胺 Caprolactan	105-60-2	NA	NA	NA
24	克菌丹 Captan	133-06-2	NA	0.60	1.52 - 4.10
25	西维因 Carbaryl	63-25-2	NA	4.48 x 10 ⁻⁵ - 1.287	1.59 - 3.13

Table E.1. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
26	二硫化碳 Carbon disulfide	75-15-0	1.3 x 10 ³ - 2.3 x 10 ³	NA	NA
27	四氯化碳 Carbon tetrachloride	56-23-5	2.0 x 10 ³ - 3.6 x 10 ³	2000 - 3081	2.03 - 3.00
28	硫化羰 Carbonyl sulfide	463-58-1	3.1 x 10 ³ - 6.8 x 10 ³	NA	NA
29	邻苯二酚 Catechol	120-80-9	2.2 x 10 ⁻²	0.022	0.53 - 1.28
30	氯胺 Chloramben	133-90-4	NA	0.274	-2.64 - 1.46
31	顺式氯丹 <i>cis</i> -Chlordane	5103-71-9	NA	0.248 - 570	2.78 - 6.21
32	反氯丹 <i>trans</i> -Chlordane	5103-74-2	NA	NA	NA
33	氯乙酸 Chloroacetic acid	79-11-8	9.2 x 10 ⁻⁴	NA	0.22
34	氯乙酰苯 Chloroacetophenone	532-27-4	NA	NA	NA
35	氯苯 Chlorobenzene	108-90-7	3.2 x 10 ² - 4.6 x 10 ²	263 - 545	2.13 - 3.18
36	克氯苯 Chlorobenzilate	510-15-6	NA	NA	NA
37	三氯甲烷 Chloroform	67-66-3	1.1 x 10 ² - 6.8 x 10 ²	198.0 - 536.9	1.43 - 2.22
38	氯甲基甲基醚 Chloromethyl methyl ether	107-30-2	NA	NA	NA
39	氯丁二烯 Chloroprene	126-99-8	NA	3242	2.03
40	邻甲苯酚 <i>o</i> -Cresol	95-48-7	8.4 x 10 ⁻² - 3.9 x 10 ⁻¹	0.07 - 0.284	1.95 - 2.24
41	间甲酚 <i>m</i> -Cresol	108-39-4	7.2 x 10 ⁻² , 1.6 x 10 ⁻¹	0.0203 - 0.1068	1.94 - 2.12
42	对甲酚 <i>p</i> -Cresol	106-44-5	4.1 x 10 ⁻² - 1.9 x 10 ⁻¹	0.0223 - 1.0820	1.62 - 2.20
43	乙酸辛酯 <i>o</i> -Cresyl acetate	533-18-6	NA	NA	NA
44	异丙基苯 Cumene	98-82-8	1.3 x 10 ² - 1.5 x 10 ³	909 - 1521	3.23 - 3.66
45	重氮甲烷 Diazomethane	334-88-3	NA	NA	NA
46	二苯并呋喃 Dibenzofuran	132-64-9	NA	NA	3.86 - 4.57
47	二溴氯丙烷 1,2-Dibromo-3-chloropropane	96-12-8	NA	NA	NA
48	2,4-二氯苯氧乙酸 2,4-Dichloro-phenoxyacetic acid	94-75-7	NA	1.39 x 10 ⁻⁵ - 0.55	-1.36 - 4.88 1.57 - 3.00
49	1,1-二氯-2,2-双(4-氯苯基)乙烯 1,1-Dichloro-2,2-bis(<i>p</i> -chlorophenyl)ethylene	72-55-9	NA	0.78 - 370	4.28 - 6.96
50	邻苯二甲酸二丁酯 Dibutyl phthalate	84-74-2	NA	0.0284 - 0.456	3.31 - 5.74

Table E.1. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
51	对二氯苯 1,4-Dichlorobenzene	106-46-7	64-4.6 x 10 ²	119 - 744	3.14 - 3.90
52	3,3' -二氯联苯胺 3,3'-Dichlorobenzidine	84-68-4	NA	0.0811	3.02 - 3.64
53	二氯乙醚 Dichloroethyl ether	111-44-4	2.2	1.320, 28.97	1.12 - 1.58
54	反式-1,3-二氯丙烯 <i>trans</i> -1,3-Dichloropropene	10061-02-6	1.6 x 10 ² -3.6 x 10 ²	137 - 429	1.41 - 1.98
55	2,2-二氯乙烯基二甲基磷酸酯 Dichlorvos	62-73-7	NA	0.097 - 0.194	1.16 - 2.29
56	二乙醇胺 Diethanolamine	111-42-2	NA	5.42 x 10 ⁻⁹	-1.25 - (-1.43)
57	硫酸二乙酯 Diethyl sulfate	64-67-5	NA	NA	NA
58	二乙二醇丁醚 Diethylene glycol monobutyl ether	112-34-5	NA	NA	NA
59	邻二茴香胺 3,3'-Dimethoxybenzidine	119-90-4	NA	NA	NA
60	二甲基黄 4-Dimethylamino-azobenzene	60-11-7	NA	NA	NA
61	N,N-二甲基苯胺 N,N-Dimethylaniline	121-69-7	NA	11.734	1.66 - 2.62
62	4,4'-二氨基-3,3'-二甲基联苯 3,3'-Dimethylbenzidine	119-93-7	NA	NA	NA
63	二甲氨基甲酰氯 Dimethylcarbamyl chloride	79-44-7	NA	NA	NA
64	N,N-二甲基甲酰胺 N,N-Dimethylformamide	68-12-2	NA	NA	NA
65	偏二甲胍 1,1-Dimethylhydrazine	57-14-7	NA	NA	NA
66	邻苯二甲酸二甲酯 Dimethyl phthalate	131-11-3	3.4 x 10 ⁴	0.011 - 0.218	1.47 - 3.40
67	硫酸二甲酯 Dimethyl sulfate	77-78-1	NA	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log Kow ^b
68	4,6-二硝基邻甲酚 4,6-Dinitro- <i>o</i> -cresol	534-52-1	2.2 x 10 ⁻⁴ , 4.4 x 10 ⁻²	4.050, 43.22	2.12 - 2.85
69	2,4-二硝基酚 2,4-Dinitrophenol	51-28-5	8.4 x 10 ⁻³ , 2.9 x 10 ⁻²	8.880 x 10 ⁻⁵ -0.00355	1.18 - 1.92
70	2,4-二硝基甲苯 2,4-Dinitrotoluene	121-14-2	4.8	0.0160 - 0.4560	1.85 - 2.04
71	1,4-二氧六环 1,4-Dioxane	123-91-1	0.46 - 0.72	0.431 - 1.564	-0.42 - 0.01
72	二苯肼 1,2-Diphenylhydrazine	122-66-7	NA	3.45 x 10 ⁻⁴	1.70 - 3.82
73	环氧氯丙烷,AR Epichlorohydrin	13403-37-7	3.6	3.375	0.30, 0.58
74	1,2-环氧丁烷 1,2-Epoxybutane	106-88-7	NA	NA	NA
75	丙烯酸乙酯 Ethyl acrylate	140-88-5	NA	34.041	0.66 - 1.33

Table E.1. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
76	乙基苯 Ethylbenzene	100-41-4	6.0 x 10 ² - 9.2 x 10 ²	653 - 1001	2.68 - 3.43
77	氨基甲酸乙酯 Ethyl carbamate	51-79-6	NA	NA	NA
78	乙基氯 Ethyl chloride	75-00-3	2.0 x 10 ² - 1.5 x 10 ³	860 - 1512	1.20 - 1.55
79	二溴乙烷 Ethylene dibromide	106-93-4	68 - 92	15.64 - 133.12	NA
80	1,2-二氯乙烷 Ethylene dichloride	107-06-2	92 - 1.6 x 10 ²	92.00 - 143	1.30 - 1.79
81	乙二醇 Ethylene glycol	107-21-1	2.5 x 10 ⁻⁵ , 6.0 x 10 ⁻³	0.006 - 5.81 x 10 ⁻⁶	-2.02 - (-0.54)
82	乙二醇单丁醚 Ethylene glycol monobutyl ether	111-76-2	NA	NA	NA
83	乙烯亚胺 Ethyleneimine	151-56-4	NA	NA	NA
84	环氧乙烷 Ethylene oxide	75-21-8	NA	NA	NA
85	乙烯硫脲 Ethylene thiourea	96-45-7	NA	NA	NA
86	1,1-二氯乙烷 Ethylidene dichloride	75-34-3	5.1 x 10 ² - 7.8 x 10 ²	421.4 - 594.9	1.78 - 1.92
87	甲醛 Formaldehyde	50-00-0	7.2 x 10 ⁻³ - 3.4 x 10 ⁻²	0.0169 - 0.0331	-0.75 - 0.35
88	七氯 Heptachlor	76-44-8	NA	17.8 - 233	3.87 - 5.73
89	六氯苯 Hexachlorobenzene	118-74-1	5.1 - 4.2 x 10 ⁴	5.07 - 172	4.13 - 7.42
90	六氯丁二烯 Hexachlorobutadiene	87-68-3	1.0 x 10 ³ - 2.5 x 10 ³	1044 - 2604	3.74 - 4.78
91	α-六氯环己烷(α)1,2,3,4,5,6- Hexachlorocyclohexane	60291-32-9	7.8 x 10 ⁻¹	0.43 - 2.16	3.80 - 4.44
92	γ-六氯环己烷(γ)1,2,3,4,5,6- Hexachlorocyclohexane	58-89-9	4.6 x 10 ⁻² - 3.6 x 10 ⁻¹	0.005 - 1.496	2.81 - 5.43

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
93	六氯环戊二烯 Hexachloro-cyclopentadiene	77-47-4	NA	1621 - 3668	3.99 - 5.51
94	六氯乙烷Hexachloroethane	67-72-1	1.2 x 10 ² - 2.3 x 10 ³	123.9 - 1302	2.73 - 4.62
95	1,6-己二异氰酸酯 Hexamethylene diisocyanate	822-06-0	NA	NA	NA
96	六甲基磷酰三胺 Hexamethyl-phosphoramidate	680-31-9	NA	NA	NA
97	正己烷Hexane	110-54-3	1.0 x 10 ⁵ - 1.8 x 10 ⁵	50,586 - 190,000	2.90 - 4.25
98	胼 Hydrazine	302-01-2	NA	NA	NA
99	对苯二酚Hydroquinone	123-31-9	3.9 x 10 ⁻⁶ - 6.0 x 10 ⁻⁶	3.89 x 10 ⁻⁶ - 5.91 x 10 ⁻⁶	0.47 - 1.28
100	异佛尔酮Isophorone	78-59-1	0.60	NA	NA

Table E.1. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
101	顺丁烯二酸酐 Maleic anhydride	108-31-6	NA	NA	NA
102	甲醇 Methanol	67-56-1	4.4 x 10 ⁻¹ - 7.2 x 10 ⁻¹	0.319 - 13.68	-1.27 - (-0.25)
103	甲氧氯 Methoxychlor	72-43-5	NA	0.999, 1.60	3.31 - 5.67
104	溴甲烷 Methyl bromide	74-83-9	5.3 x 10 ² - 2.3 x 10 ⁴	533 - 20,262	1.00 - 1.19
105	氯甲烷 Methyl chloride	74-87-3	7.8 x 10 ² - 3.5 x 10 ³	669 - 4052	0.81 - 1.06
106	1,1,1-三氯乙烷 Methyl chloroform	71-55-6	4.6 x 10 ² - 3.8 x 10 ³	399.9 - 3620	1.96 - 2.60
107	甲乙酮 Methyl ethyl ketone	78-93-3	4.8 - 25	1.064 - 13.17	-0.27 - 0.785
108	甲基胍 Methylhydrazine	60-34-4	NA	NA	NA
109	碘甲烷 Methyl iodide	74-88-4	2.9 x 10 ² - 7.2 x 10 ²	278.1 - 554.9	1.50 - 1.69
110	4-甲基-2-戊酮 Methyl isobutyl ketone	108-10-1	19 - 46	9.523, 39.52	1.09 - 1.31
111	异氰酸甲酯 Methyl isocyanate	624-83-9	NA	NA	NA
112	甲基丙烯酸甲酯 Methyl methacrylate	80-62-6	NA	24.310 - 32.823	0.67 - 1.38
113	甲基叔丁基醚 Methyl tert-butyl ether	1634-04-4	60, 63	59.46 - 305	0.94 - 1.30
114	4,4'-二氨基-3,3'-二氯二苯甲烷 4,4'-Methylenebis(2-chloroaniline)	101-14-4	NA	NA	NA
115	二氯甲烷 Methylene chloride	75-09-2	84 - 3.3 x 10 ²	173.0 - 451.1	1.01 - 1.63
116	4,4'-亚甲基双(异氰酸苯酯) 4,4'-Methylenediphenyl diisocyanate	101-68-8	NA	NA	NA
117	4,4'-二氨基二苯甲烷 4,4'-Methylenedianiline	101-77-9	NA	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log Kow ^b
118	萘 Naphthalene	91-20-3	42 - 1.3 x 10 ²	29.2 - 123.95	3.01 - 4.70
119	硝基苯 Nitrobenzene	98-95-3	2.2 - 2.5	1.327 - 4.723	1.60 - 2.93
120	4-硝基联苯 4-Nitrobiphenyl	92-93-3	NA	NA	NA
121	4-硝基苯酚 4-Nitrophenol	100-02-7	3.8 x 10 ⁻⁷ - 1.0 x 10 ⁻³	1.04 x 10 ⁻⁵ - 2.533	0.70 - 2.91
122	2-硝基丙烷 2-Nitropropane	79-46-9	9.2, 12	NA	NA
123	甲基-1-亚硝基脲 N-Nitroso-N-methylurea	684-93-5	NA	NA	NA
124	N-亚硝基二甲胺 N-Nitrosodimethylamine	62-75-9	NA	3.344	-0.68 - 0.76
125	N-亚硝基吗啉 N-Nitrosomorpholine	59-89-2	NA	NA	NA

Table E.1. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
126	乙基对硫磷 Parathion	56-38-2	1.2 x 10 ⁻¹	0.012 - 0.120	2.15 - 4.00
127	五氯硝基苯 Pentachloro-nitrobenzene	82-68-8	NA	0.3718 - 0.4812	4.22 - 6.0
128	五氯酚 Pentachlorophenol	87-86-5	2.5 x 10 ⁻³ - 9.2	0.0025 - 0.2840	2.50 - 5.86
129	苯酚 Phenol	108-95-2	3.4 x 10 ⁻² - 1.3 x 10 ³	0.0274 - 1.0820	0.62 - 2.20
130	对苯二胺 <i>p</i> -Phenylenediamine	106-50-3	NA	NA	NA
131	氯代甲酰氯 Phosgene	75-44-5	NA	NA	NA
132	磷化氢 Phosphine	7803-51-2	1.3 x 10 ⁴	NA	NA
133	苯酐 Phthalic anhydride	85-44-9	NA	NA	NA
134	1,3-丙烷磺内酯 1,3-Propane sultone	1120-71-4	NA	NA	NA
135	β-丙内酯 β-Propiolactone	57-57-8	NA	NA	NA
136	丙醛 Propionaldehyde	123-38-6	7.8 - 36	7.436 - 13.77	0.00 - 0.83
137	2-(1-甲基乙氧基)苯基氨基甲酸酯 Propoxur	114-26-1	NA	1.98 x 10 ⁻⁶ - 0.1308	1.45 - 2.01
138	1,2-Dichloropropane	26198-63-0	2.5 x 10 ² - 3.4 x 10 ²	31.21 - 2261	1.99 - 2.30
139	环氧丙烷 Propylene oxide	75-56-9	19	8.653	0.03 - 0.23
140	2-甲基氮丙啶 1,2-Propylenimine	75-55-8	NA	NA	NA
141	喹啉 Quinoline	91-22-5	2.7 x 10 ⁻²	0.0253 - 0.1680	1.88 - 2.10
142	苯醌 Quinone	106-51-4	NA	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log Kow ^b
143	苯乙烯 Styrene	100-42-5	2.7 x 10 ² - 3.5 x 10 ²	233 - 527	2.76 - 3.39
144	氧化苯乙烯 Styrene oxide	96-09-3	NA	NA	1.43 - 1.84
145	2,3,7,8-四氯二苯并对-二噁英 (硫丙磷) 2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	1746-01-6	NA	0.0021 - 10.34	5.38 - 8.93
146	四氯乙烷 1,1,2,2-Tetrachloroethane	79-34-5	34 - 56	25.33 - 48.6	2.39 - 3.27
147	四氯乙烯 Tetrachloroethylene	127-18-4	8.4 x 10 ² - 3.0 x 10 ³	248 - 2940	NA
148	甲苯 Toluene	108-88-3	4.8 x 10 ² - 7.8 x 10 ²	518 - 825	1.83 - 3.06
149	2,4-二氨基甲苯 Toluene-2,4-diamine	95-80-7	NA	NA	NA
150	2,4-甲苯二异氰酸酯 2,4-Toluene diisocyanate	584-84-9	NA	NA	NA

Table E.1. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
151	邻甲苯胺 o-Toluidine	95-53-4	NA	0.095	1.29 - 1.63
152	氯代萘烯 Toxaphene	8001-35-2	NA	0.0238 - 6382	2.92 - 5.50
153	三氯苯 1,2,4-Trichlorobenzene	120-82-1	1.4 x 10 ² - 3.8 x 10 ²	101 - 435	3.34 - 4.40
154	1,1,2-三氯乙烷 1,1,2-Trichloroethane	79-00-5	78 - 1.2 x 10 ²	70.92 - 120	1.89 - 2.42
155	三氯乙烯 Trichloroethylene	79-01-6	4.2 x 10 ² - 1.4 x 10 ³	119 - 1215	2.04 - 3.57
156	2,4,5-三氯苯酚 2,4,5-Trichlorophenol	95-95-4	NA	0.521, 0.590	2.39 - 4.19
157	2,4,6-三氯酚 2,4,6-Trichlorophenol	88-06-2	NA	0.405, 0.5687	2.67 - 4.03
158	三乙胺 Triethylamine	121-44-8	15	NA	NA
159	2,6-二硝基-N,N-二正丙基-4-三氟甲基苯 胺 (氟乐灵) Trifluralin	1582-09-8	NA	4.02 - 16.61	3.0 - 5.34
160	2,2,4-三甲基戊烷 2,2,4-Trimethylpentane	540-84-1	NA	110,669 - 472,092	4.06 - 5.83
161	醋酸乙烯酯 Vinyl acetate	108-05-4	60	48.74	0.21 - 0.73
162	溴乙烯 Vinyl bromide	593-60-2	NA	NA	NA
163	氯乙烯 Vinyl chloride	75-01-4	2.2 x 10 ³ - 1.2 x 10 ⁵	494.6 - 8246	0.60 - 1.39
164	过氯乙烯 Vinylidene chloride	75-35-4	1.5 x 10 ³ - 1.9 x 10 ⁴	NA	NA
165	邻二甲苯 o-Xylene	95-47-6	3.5 x 10 ² - 5.3 x 10 ²	429 - 895	2.12 - 3.42
166	间二甲苯 m-Xylene	108-38-3	6.0 x 10 ² - 7.8 x 10 ²	506 - 1115	3.04 - 3.50
167	对二甲苯 p-Xylene	106-42-3	4.4 x 10 ² - 8.4 x 10 ²	506 - 1185	3.06 - 3.50

^aSander (1999)

^bMackay et al. (1992a and b, 1993, 1995)

^cNA, not available

Table E.2. Range of reported values of H and log K_{ow} for polychlorinated byphenyls (PCB) congeners at 293-298 K.

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
1	2-氯联苯 2-Monochloro	2051-60-7	NA ^e	20.43 - 30.2	28.9 - 74.6	3.75 - 5.70
2	3-氯联苯 3-Monochloro	2051-61-8	NA	29.0	14.49 - 75.5	4.34 - 4.95
3	4-氯联苯 4-Monochloro	2051-62-9	NA	27.8	24.39 - 58.06	4.26 - 4.94
4	2,2'-二氯联苯 2,2'-Dichloro	13029-08-8	23 - 56	23, 33.3	22.29 - 59.17	3.55 - 5.70
5	2,3-二氯联苯 2,3-Dichloro	16605-91-7	NA	23, 24.2	19.56 - 28.57	4.97 - 5.36
6	2,3'-二氯联苯 2,3'-Dichloro	25569-80-6	NA	25, 33.1	NA	NA
7	2,4-二氯联苯 2,4-Dichloro	33284-50-3	NA	28, 38.2	24.78 - 96.66	4.67 - 5.30
8	2,4'-二氯联苯 2,4'-Dichloro	34883-43-7	NA	20.3 - 30.7	22.29 - 96.7	4.47 - 5.51
9	2,5-二氯联苯 2,5-Dichloro	34883-39-1	34 - 44	32.8	20.1 - 39.31	4.67 - 5.46
10	2,6-二氯联苯 2,6-Dichloro	33146-45-1	NA	42.9	47.61 - 47.83	4.05 - 5.46
11	3,3-二氯联苯 3,3'-Dichloro	2050-67-1	14, 24	29.4	13.58 - 23.61	5.10 - 5.34
12	3,4-二氯联苯 3,4-Dichloro	2974-92-7	10, 21	14, 23.7	9.60 - 20.77	5.05 - 5.51
13	3,4'-二氯联苯 3,4'-Dichloro	2974-90-5	NA	25.7	NA	NA
14	3,5-二氯联苯 3,5-Dichloro	34883-41-5	NA	42.6	16.72 - 49.55	5.10 - 5.41
15	4,4'-二氯联苯 4,4'-Dichloro	2050-68-2	11 - 31	22.7	9.66 - 30.4	4.77 - 5.58
16	2,2',3-三氯联苯 2,2',3-Trichloro	38444-78-9	NA	20, 25.5	20.27 - 81.77	4.15 - 5.60
17	2,2,4-三氯联苯 2,2',4-Trichloro	37680-66-3	NA	37.8	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
18	2,2,5-三氯联苯醚 2,2',5-Trichloro	37680-65-2	NA	25.3 - 58.1	20.26 - 101.53	3.89 - 6.22
19	2,2,6-三氯联苯 2,2',6-Trichloro	38444-73-4	NA	23, 44.7	NA	NA
20	2,3,3'-三氯联苯 2,3,3'-Trichloro	38444-84-7	NA	16, 22.0	16.21 - 82.0	4.99 - 5.60
21	2,3,4-三氯联苯醚 2,3,4-Trichloro	55702-46-0	NA	23.0	14.79 - 21.38	5.39 - 5.88
22	2,3,4'-三氯联苯 2,3,4'-Trichloro	38444-85-8	NA	14, 19.4	NA	NA
23	2,3,5-三氯联苯 2,3,5-Trichloro	55720-44-0	NA	32.3	NA	NA
24	2,3,6-三氯联苯 2,3,6-Trichloro	58702-45-9	NA	22, 31.5	NA	NA
25	2,3',4-三氯联苯 2,3',4-Trichloro	55712-37-3	NA	32.0	NA	NA

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
26	2,3',5-三氯联苯 2,3',5-Trichloro	38444-81-4	29, 34	20, 30.2	20.27 - 34.34	5.18 - 5.88
27	2,3',6-三氯联苯 2,3',6-Trichloro	38444-76-7	NA	41.0	NA	NA
28	2,4,4'-三氯联苯 2,4,4'-Trichloro	7012-37-5	28	20.3 - 38.14	20.27 - 33.0	5.11 - 6.00
29	2,4,5-三氯联苯 2,4,5-Trichloro	15862-07-4	NA	20.3 - 37.89	20.27 - 27.05	5.22 - 6.25
30	2,4,6-三氯联苯 2,4,6-Trichloro	35693-92-6	0.72 - 68	58.0	49.51 - 65.76	5.44 - 6.17
31	2,4,5-三氯联苯醚 2,4',5-Trichloro	16606-02-3	NA	19, 27.8	19.25 - 94.13	5.11 - 6.22
32	2,4',6-三氯联苯 2,4',6-Trichloro	38444-77-8	NA	39.7	NA	NA
33	2',3,4-三氯联苯 2',3,4-Trichloro	38444-86-9	NA	24.3	15.20 - 43.67	5.46 - 6.10
34	2',3,5-三氯联苯 2',3,5-Trichloro	37680-68-5	NA	42.7	NA	NA
35	3,3',4-三氯联苯 3,3',4-Trichloro	37680-69-6	NA	18.2	8.13 - 22.49	5.53 - 5.82
36	3,3',5-三氯联苯 3,3',5-Trichloro	38444-87-0	NA	17, 34.1	NA	NA
37	3,4,4'-三氯联苯 3,4,4'-Trichloro	38444-90-5	NA	10, 15.4	7.34 - 84.21	4.94 - 6.00
38	3,4,5-三氯联苯 3,4,5-Trichloro	53555-66-1	NA	23.5	NA	NA
39	3,4',5-三氯联苯 3,4',5-Trichloro	38444-88-1	NA	30.3	NA	NA
40	2,2',3,3'-四氯联苯 2,2',3,3'-Tetrachloro	38444-93-8	12, 21	10, 18.5	10.13 - 21.94	4.54 - 6.67
41	2,2',3,4-四氯联苯 2,2',3,4-Tetrachloro	52663-59-9	NA	14, 24.8	NA	NA
42	2,2',3,4'-四氯联苯 2,2',3,4'-Tetrachloro	36559-22-5	NA	14, 25.9	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
43	2,2',3,5-四氯联苯 2,2',3,5-Tetrachloro	70362-46-8	NA	33.9	NA	NA
44	2,2',3,5'-四氯联苯 2,2',3,5'-Tetrachloro	41464-39-5	NA	23.3 - 32.8	19.15 - 79.28	4.79 - 6.67
45	2,2',3,6-四氯联苯 2,2'3,6-Tetrachloro	70362-45-7	NA	36.0	NA	NA
46	2,2',3,6'-四氯联苯 2,2',3,6'-Tetrachloro	41464-47-5	NA	34.3	NA	NA
47	2,2',4,4'-四氯联苯 2,2',4,4'-Tetrachloro	2437-79-8	NA	19, 37.3	17.38 - 44.48	5.20 - 7.13
48	2,2',4,5-四氯联苯 2,2',4,5-Tetrachloro	70362-47-9	NA	30.7	NA	NA
49	2,2',4,5'-四氯联苯 2,2',4,5'-Tetrachloro	41464-40-8	NA	21, 35.8	20.27 - 47.72	5.20 - 6.88
50	2,2',4,6-四氯联苯 2,2',4,6- Tetrachloro	62796-65-8	NA	61.8 - 138	58.57 - 137.8	5.63 - 5.96

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
51	2,2',4,6'-四氯联苯 2,2',4,6'-Tetrachloro	65194-04-7	NA	51.7	49.04 - 101.2	5.51 - 5.96
52	2,2,5,5-四氯联苯 2,2',5,5'-Tetrachloro	35693-99-3	2.5 - 53	20 - 53.2	2.53 - 160	3.91 - 6.90
53	2,2',5,6'-四氯联苯 2,2',5,6'- Tetrachloro	41464-41-9	26, 42	43.6	28.67 - 112.5	5.46 - 5.96
54	2,2',6,6'-四氯联苯 2,2',6,6'- Tetrachloro	15968-05-5	15 - 190	20, 58.0	15.0 - 188.5	4.16 - 7.13
55	2,3,3',4-四氯联苯 2,3,3',4-Tetrachloro	74338-24-2	NA	18.5	NA	NA
56	2,3,3',4'-四氯联苯 2,3,3',4'-Tetrachloro	41464-43-1	NA	15.3	NA	NA
57	2,3,3',5-四氯联苯 2,3,3',5-Tetrachloro	70424-67-8	NA	27.4	NA	NA
58	2,3,3',5'-四氯联苯 2,3,3',5'-Tetrachloro	41464-49-7	NA	25.3	NA	NA
59	2,3,3',6-四氯联苯 2,3,3',6-Tetrachloro	74472-33-6	NA	30.8	NA	NA
60	2,3,4,4'-四氯联苯 2,3,4,4'-Tetrachloro	33025-41-1	NA	15.5	10.34 - 84.20	5.33 - 6.25
61	2,3,4,5-四氯联苯 2,3,4,5-Tetrachloro	33284-53-6	NA	24.1	11.45 - 17.53	5.72 - 6.88
62	2,3,4,6-Tetrachloro	54230-23-7	NA	21, 37.5	NA	NA
63	2,3,3',4,6-五氯联苯 2,3,4',5-Tetrachloro	74472-35-8	NA	24.6	NA	NA
64	2,3,4',6-四氯联苯 2,3,4',6-Tetrachloro	52663-58-8	NA	27.6	NA	NA
65	2,3,5,6-四氯联苯 2,3,5,6-Tetrachloro	33284-54-7	NA	34.1	NA	NA
66	2,3',4,4'-四氯联苯 2,3',4,4'-Tetrachloro	32598-10-0	NA	13.7 - 84.2	13.68 - 84.20	5.45 - 6.67
67	2,3",4,5-四氯联苯 2,3',4,5-Tetrachloro	73575-53-8	NA	10, 23.7	NA	NA
68	2,3',4,5'-四氯联苯 2,3',4,5'-Tetrachloro	73575-52-7	NA	38.2	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
69	2,3',4,6-四氯联苯 2,3',4,6-Tetrachloro	60233-24-1	NA	51.3	NA	NA
70	2,3,4,5-四氯联苯醚 2,3',4',5-Tetrachloro	32598-11-1	NA	10, 20.5	10.13 - 20.26	5.20 - 7.13
71	2,3',4',6-四氯联苯 2,3',4',6-Tetrachloro	41464-46-4	NA	31.8	NA	NA
72	2,4',5,5'-四氯联苯 2,4',5,5'-Tetrachloro	41464-42-0	NA	36.7	NA	NA
73	2,3',5',6-四氯联苯 2,3',5',6-Tetrachloro	74338-23-1	NA	52.7	NA	NA
74	2,4,4',5-四氯联苯 2,4,4',5-Tetrachloro	32690-93-0	NA	10, 21.8	NA	NA
75	2,4,4',6-四氯联苯 2,4,4',6-Tetrachloro	32598-12-2	NA	47.1	42.25 - 55.32	5.87 - 6.05

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
76	2',3,4,5-四氯联苯 2',3,4,5-Tetrachloro	70362-48-0	NA	24.2	NA	NA
77	3,3,4,4-四氯联苯 3,3',4,4'-Tetrachloro	32598-13-3	4.4, 9.2	4.37 - 16.2	1.72 - 9.52	5.27 - 6.77
78	3,3',4,5-四氯联苯 3,3'4,5-Tetrachloro	70362-49-1	NA	16.5	NA	NA
79	3,3',4,5'-四氯联苯 3,3',4,5'-Tetrachloro	41464-48-6	NA	20.0	NA	NA
80	3,3',5,5'-四氯联苯 3,3',5,5'-Tetrachloro	33284-52-5	NA	38.0	12.46 - 63.02	6.05 - 6.85
81	3,4,4',5-四氯联苯 3,4,4',5-Tetrachloro	70362-50-4	NA	14.5	NA	NA
82	2,2',3,3',4-五氯联苯 2,2',3,3',4-Pentachloro	52663-62-4	NA	14.8	NA	NA
83	2,2',3,3',5-五氯联苯 2,2',3,3',5-Pentachloro	60145-20-2	NA	21.5	16.62 - 26.65	6.24 - 6.26
84	2,2',3,3',6-戊氯联苯 2,2',3,3',6-Pentachloro	52663-60-2	NA	25.5	NA	NA
85	2,2',3,4,4'-五氯联苯醚 2,2',3,4,4'-Pentachloro	65510-45-4	NA	6.7, 19.5	NA	NA
86	2,2',3,4,5-戊氯联苯 2,2',3,4,5-Pentachloro	55312-69-1	NA	24.1	17.23 - 84.1	6.20 - 7.49
87	2,2',3,4,5'-戊氯联苯 2,2',3,4,5'-Pentachloro	38380-02-8	NA	7.5 - 37.71	7.50 - 33.44	5.45 - 7.43
88	2,2',3,4,6-戊氯联苯 2,2',3,4,6-Pentachloro	55215-17-3	NA	39.0	34.65 - 136.8	6.07 - 7.51
89	2,2',3,4,6'-五氯联苯 2,2',3,4,6'-Pentachloro	73575-57-2	NA	30.2	NA	NA
90	2,2',3,4',5-戊氯联苯 2,2',3,4',5-Pentachloro	68194-07-0	NA	29.8	NA	NA
91	2,2',3,4',6-戊氯联苯 2,2',3,4',6-Pentachloro	58194-05-8	NA	35.1	NA	NA
92	2,2',3,5,5'-戊氯联苯 2,2',3,5,5'-Pentachloro	52663-61-3	NA	26.3	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
93	2,2',3,5,6-戊氯联苯 2,2',3,5,6-Pentachloro	73575-56-1	NA	34.5	NA	NA
94	2,2',3,5,6'-戊氯联苯 2,2',3,5,6'-Pentachloro	73575-55-0	NA	39.7	NA	NA
95	2,2',3,5',6-戊氯联苯 2,2',3,5',6-Pentachloro	38379-99-6	NA	12, 30.4	20.06 - 82.78	5.18 - 6.55
96	2,2',3,6,6'-戊氯联苯 2,2',3,6,6'-Pentachloro	73575-54-9	NA	41.6	NA	NA
97	2,2',3',4,5-戊氯联苯 2,2',3',4,5-Pentachloro	41464-51-1	NA	7.5, 18.2	NA	NA
98	2,2',3',4,6-五氯联苯 2,2',3',4,6- Pentachloro	60233-25-2	NA	39.7	NA	NA
99	2,2',4,4',5-五氯联苯 2,2',4,4',5-Pentachloro	38380-01-7	NA	7.9, 25.3	7.90 - 30.50	6.11 - 7.21
100	2,2',4,4',6-戊氯联苯 2,2',4,4',6-Pentachloro	39485-83-1	NA	57.0	62.62 - 97.27	5.5 - 6.44

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
101	2,2,4,5,5-五氯联苯 2,2',4,5,5'-Pentachloro	37680-73-2	7.2-33	9.1 - 42.07	7.09 - 35.48	4.12 - 7.64
102	2,2',4,5,6'-五氯联苯 2,2',4,5,6'-Pentachloro	68194-06-9	NA	9.1, 37.6	NA	NA
103	2,2',4,5',6-五氯联苯 2,2',4,5',6-Pentachloro	60145-21-3	NA	51.0	NA	NA
104	2,2',4,6,6'-五氯联苯 2,2',4,6,6'-Pentachloro	56558-16-8	92, 180	66.0 - 185	90.9 - 185.4	5.37 - 6.40
105	2,3,3,4,4-五氯二苯酚 2,3,3',4,4'-Pentachloro	32598-14-4	NA	5.68 - 33.6	NA	NA
106	2,3,3',4,5-五氯联苯 2,3,3',4,5-Pentachloro	70424-69-0	NA	16.7	NA	NA
107	2,3,3',4',5-五氯联苯 2,3,3',4',5-Pentachloro	70424-68-9	NA	16.1	NA	NA
108	2,3,3',4,5'-五氯联苯 2,3,3',4,5'-Pentachloro	70362-41-3	NA	17.8	NA	NA
109	2,3,3',4,6-五氯联苯 2,3,3',4,6-Pentachloro	74472-35-8	NA	28.6	NA	NA
110	2,3,3',4',6-五氯联苯 2,3,3',4',6-Pentachloro	38380-03-9	NA	19.9	10.74 - 37.48	6.20 - 6.53
111	2,3,3',5,5'-五氯联苯 2,3,3',5,5'-Pentachloro	39635-32-0	NA	27.0	NA	NA
112	2,3,3',5,6-五氯联苯 2,3,3',5,6-Pentachloro	74472-36-9	NA	27.0	NA	NA
113	2,3,3',5',6-五氯联苯 2,3,3',5',6-Pentachloro	68194-10-5	NA	33.0	NA	NA
114	2,3,4,4',5-五氯联苯 2,3,4,4',5-Pentachloro	74472-37-0	NA	14.5	NA	NA
115	2,3,4,4',6-五氯联苯 2,3,4,4',6-Pentachloro	74472-38-1	NA	24.9	NA	NA
116	2,3,4,5,6-五氯联苯 2,3,4,5,6-Pentachloro	18259-05-7	NA	30.0	18.34 - 23.41	6.14 - 7.60
117	2,3,4',5,6-五氯联苯 2,3,4',5,6-Pentachloro	68194-11-6	NA	24.4	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log Kow ^b
118	2,3'4,4',5-五氯联苯 2,3'4,4',5-Pentachloro	31508-00-6	NA	9.35 - 40.5	NA	NA
119	2,3',4,4',6-五氯联苯 2,3',4,4',6-Pentachloro	56558-17-9	NA	31.5	NA	NA
120	2,3',4,5,5'-五氯联苯 2,3',4,5,5'-Pentachloro	68194-12-7	NA	5.7, 24.9	NA	NA
121	2,3',4,5',6-五氯联苯 2,3',4,5',6-Pentachloro	56558-18-0	NA	56.6	NA	NA
122	2',3,3',4,5-五氯联苯 2',3,3',4,5-Pentachloro	76842-07-4	NA	12.7	NA	NA
123	2',3,4,4',5-五氯联苯 2',3,4,4',5-Pentachloro	65510-44-3	NA	17.6	NA	NA
124	2',3,4,5,5'-五氯联苯 2',3,4,5,5'-Pentachloro	70424-70-3	NA	17.3	NA	NA
125	2',3,4,5,6'-五氯联苯 2',3,4,5,6'-Pentachloro	74472-39-2	NA	29.2	NA	NA

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
126	3,3',4,4',5-五氯联苯 3,3',4,4',5-Pentachloro	57465-28-8	NA	2.78 - 21.02	NA	NA
127	3,3',4,5,5'-五氯联苯 3,3',4,5,5'-Pentachloro	39635-33-1	NA	15.8	NA	NA
128	2,2',3,3',4,4'-六氯联苯 2,2',3,3',4,4'-Hexachloro	38380-07-3	3.1-51	1.3 - 50.7	1.32 - 50.66	6.14 - 8.31
129	2,2',3,3',4,5--六氯联苯 2,2',3,3',4,5-Hexachloro	55215-18-4	NA	2.9, 14.2	2.94 - 39.52	6.50 - 8.26
130	2,2',3,3',4,5'-六氯联苯 2,2',3,3',4,5'- Hexachloro	52663-66-8	NA	3.7, 15.4	NA	NA
131	2,2',3,3',4,6-六氯联苯 2,2',3,3',4,6- Hexachloro	61798-70-7	NA	4.0, 24.5	NA	NA
132	2,2',3,3',4,6'-六氯联苯 2,2',3,3',4,6'-Hexachloro	38380-05-1	NA	4.5, 20.5	NA	NA
133	2,2',3,3',5,5'-六氯联苯 2,2',3,3',5,5'- Hexachloro	35694-04-3	NA	20.6	NA	NA
134	2,2',3,3',5,6-六氯联苯 2,2',3,3',5,6- Hexachloro	52704-70-8	NA	5.0, 23.3	4.96 - 57.76	6.20 - 8.31
135	2,2',3,3',5,6'-六氯联苯 2,2',3,3',5,6'-Hexachloro	52744-13-5	NA	5.7, 27.2	NA	NA
136	2,2',3,3',6,6'-六氯联苯 2,2',3,3',6,6'-Hexachloro	38411-22-2	NA	8.9, 32.6	8.92 - 93.22	4.91 - 8.35
137	2,2',3,4,4',5-六氯联苯 2,2',3,4,4',5- Hexachloro	35694-06-5	NA	18.8	NA	NA
138	2,2',3,4,4',5'-六氯联苯 2,2',3,4,4',5'-Hexachloro	35065-28-2	NA	2.1 - 48.6	2.13 - 69.0	6.50 - 7.44
139	2,2',3,4,4',6-六氯联苯 2,2',3,4,4',6- Hexachloro	56030-56-9	NA	33.3	NA	NA
140	2,2',3,4,4',6'-六氯联苯 2,2',3,4,4',6'-Hexachloro	59291-64-4	NA	31.2	NA	NA
141	2,2',3,4,5,5'-六氯联苯 2,2',3,4,5,5'- Hexachloro	52712-04-6	NA	2.3, 17.6	NA	NA
142	2,2',3,4,5,6-六氯联苯 2,2',3,4,5,6- Hexachloro	41411-61-4	NA	31.9	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log Kow ^b
143	2,2',3,4,5,6'-六氯联苯 2,2',3,4,5,6'-Hexachloro	68194-15-0	NA	29.8	NA	NA
144	2,2',3,4,5',6-六氯联苯 2,2',3,4,5',6-Hexachloro	68194-14-9	NA	30.0	NA	NA
145	2,2',3,4,6,6'-六氯联苯 2,2',3,4,6,6'-Hexachloro	74472-40-5	NA	47.6	NA	NA
146	2,2',3,4',5,5'-六氯联苯 2,2',3,4',5,5'-Hexachloro	51908-16-8	NA	2.5, 19.0	NA	NA
147	2,2',3,4',5,6-六氯联苯 2,2',3,4',5,6-Hexachloro	68194-13-8	NA	5.2, 32.0	NA	NA
148	2,2',3,4',5,6'-六氯联苯 2,2',3,4',5,6'-Hexachloro	74472-42-7	NA	43.5	NA	NA
149	2,2',3,4',5',6-六氯联苯 2,2',3,4',5',6-Hexachloro	38380-04-0	NA	24.0	NA	NA
150	2,2',3,4',6,6'-六氯联苯 2,2',3,4',6,6'-Hexachloro	68194-08-1	NA	51.3	NA	NA

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
151	2,2',3,5,5',6-六氯联苯 2,2',3,5,5',6-Hexachloro	52663-63-5	NA	6.0, 28.7	NA	NA
152	2,2',3,5,6,6'-六氯联苯 2,2',3,5,6,6'-Hexachloro	68194-09-2	NA	43.3	NA	NA
153	2,2',4,4',5,5'-六氯联苯 2,2',4,4',5,5'-Hexachloro	35065-27-1	NA	2.3 - 52.8	2.33 - 224	6.34 - 8.35
154	2,2',4,4',5,6'-六氯联苯 2,2',4,4',5,6'-Hexachloro	60145-22-4	NA	38.7 - 76.7	NA	NA
155	2,2',4,4',6,6'-六氯联苯 2,2',4,4',6,6'-Hexachloro	33979-03-2	12-160	85.2	11.65 - 817.9	6.01 - 8.31
156	2,3,3',4,4',5-六氯联苯 2,3,3',4,4',5-Hexachloro	38380-08-4	6.3-36	8.97	NA	NA
157	2,3,3',4,4',5'-六氯联苯 2,3,3',4,4',5'-Hexachloro	69782-90-7	NA	8.56	NA	NA
158	2,3,3',4,4',6-六氯联苯 2,3,3',4,4',6-Hexachloro	74472-42-7	NA	16.7	NA	NA
159	2,3,3',4,5,5'-六氯联苯 2,3,3',4,5,5'-Hexachloro	39635-35-3	NA	2.0, 15.8	NA	NA
160	2,3,3',4,5,6-六氯联苯 2,3,3',4,5,6-Hexachloro	41411-62-5	NA	2.0, 21.7	NA	NA
161	2,3,3',4,5',6-六氯联苯 2,3,3',4,5',6-Hexachloro	74472-43-8	NA	28.9	NA	NA
162	2,3,3',4',5,5'-六氯联苯 2,3,3',4',5,5'-Hexachloro	39635-34-2	NA	13.3	NA	NA
163	2,3,3',4',5,6-六氯联苯 2,3,3',4',5,6-Hexachloro	74472-44-9	NA	1.5, 16.8	NA	NA
164	2,3,3',4',5',6--六氯联苯 2,3,3',4',5',6--Hexachloro	74472-45-0	NA	17.9	NA	NA
165	2,3,3',5,5',6-六氯联苯 2,3,3',5,5',6-Hexachloro	74472-46-1	NA	2.9, 27.9	NA	NA
166	2,3,4,4',5,6-六氯联苯 2,3,4,4',5,6-Hexachloro	41411-63-6	NA	18.7	NA	NA
167	2,3',4,4',5,5'-六氯联苯 2,3',4,4',5,5'-Hexachloro	52663-72-6	NA	11.1	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
168	2,3',4,4',5',6-六氯联苯 2,3',4,4',5',6-Hexachloro	59291-65-5	NA	28.0	NA	NA
169	3,3',4,4',5,5'-六氯联苯 3,3',4,4',5,5'-Hexachloro	32774-16-6	NA	6.60	1.57 - 5.98	6.64 - 7.55
170	2,2,3,3,4,4,5-七氯联苯 2,2',3,3',4,4',5-Heptachloro	35065-30-6	NA	0.91 - 20.84	0.91 - 19.25	7.03 - 7.27
171	2,2',3,3',4,4',6-七氯联苯 2,2',3,3',4,4',6-Heptachloro	52663-71-5	NA	17.5	5.40 - 29.79	6.68 - 9.03
172	2,2',3,3',4,5,5'--七氯联苯 2,2',3,3',4,5,5'-Heptachloro	52663-74-8	NA	1.3, 12.1	NA	NA
173	2,2',3,3',4,5,6--七氯联苯 2,2',3,3',4,5,6-Heptachloro	68194-16-1	NA	1.4, 18.5	NA	NA
174	2,2',3,3',4,5,6'--七氯联苯 2,2',3,3',4,5,6'-Heptachloro	38411-25-5	NA	1.4, 17.1	NA	NA
175	2,2',3,3',4,5',6--七氯联苯 2,2',3,3',4,5',6-Heptachloro	40186-70-7	NA	22.6	NA	NA

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
176	2,2',3,3',4,5',6-七氯联苯 2,2',3,3',4,6,6'-Heptachloro	52663-65-7	NA	30.1	NA	NA
177	2,2',3,3',4,5',6-七氯联苯 2,2',3,3',4',5,6-Heptachloro	52663-70-4	NA	16.5	NA	NA
178	2,2',3,3',4,5',6-七氯联苯 2,2',3,3',5,5',6-Heptachloro	52663-67-9	NA	2.3, 21.6	NA	NA
179	2,2',3,3',4,5',6-七氯联苯 2,2',3,3',5,6,6'-Heptachloro	52663-64-6	NA	2.4, 27.9	NA	NA
180	2,2',3,3',4,5',6-七氯联苯 2,2',3,4,4',5,5'-Heptachloro	35065-29-3	NA	1.01 - 37.0	1.013 - 102	6.70 - 7.36
181	2,2',3,3',4,5',6-七氯联苯 2,2',3,4,4',5,6-Heptachloro	74472-47-2	NA	23.3	NA	NA
182	2,2',3,3',4,5',6-七氯联苯 2,2',3,4,4',5,6'-Heptachloro	60145-23-5	NA	26.0	NA	NA
183	2,2',3,3',4,5',6-七氯联苯 2,2',3,4,4',5',6-Heptachloro	52663-69-1	NA	20.4	NA	NA
184	2,2',3,3',4,5',6-七氯联苯 2,2',3,4,4',6,6'-Heptachloro	74472-48-3	NA	46.4	NA	NA
185	2,2',3,3',4,5',6-七氯联苯 2,2',3,4,5,5',6- Heptachloro	52712-05-7	NA	1.6, 21.7	1.62 - 46.0	6.99 - 8.94
186	2,2',3,3',4,5',6--七氯联苯 2,2',3,4,5,6,6'-Heptachloro	74472-49-4	NA	37.3	NA	NA
187	2,2',3,3',4,5',6--七氯联苯 2,2',3,4',5,5',6-Heptachloro	52663-68-0	NA	20.5 - 62.2	8.41 - 42.15	6.92 - 7.19
188	2,2',3,4',5,6,6'-七氯联苯 2,2',3,4',5,6,6'-Heptachloro	74487-85-7	NA	44.9 - 113	NA	NA
189	2,3,3',4,4',5,5'-七氯联苯 2,3,3',4,4',5,5'-Heptachloro	39635-31-9	NA	6.74	NA	NA
190	2,3,3',4,4',5,6-七氯联苯 2,3,3',4,4',5,6-Heptachloro	41411-64-7	NA	11.4	NA	NA
191	2,3,3',4,4',5',6-七氯联苯 2,3,3',4,4',5',6-Heptachloro	74472-50-7	NA	13.5	NA	NA
192	2,3,3',4,5,5',6-七氯联苯 2,3,3',4,5,5',6-Heptachloro	74472-51-8	NA	19.4	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
193	2,3,3',4',5,5',6-七氯联苯 2,3,3',4',5,5',6-Heptachloro	69782-91-8	NA	13.6	NA	NA
194	2,2',3,3',4,4',5,5'-八氯联苯 2,2',3,3',4,4',5,5'-Octachloro	35694-08-7	NA	1.0, 6.79	10.13 - 47.52	6.90 - 9.69
195	2,2',3,3',4,4',5,6-八氯联苯 2,2',3,3',4,4',5,6-Octachloro	52663-78-2	NA	1.1 - 14.13	NA	NA
196	2,2',3,3',4,4',5,6'-八氯联苯 2,2',3,3',4,4',5,6'-Octachloro	42740-50-1	NA	1.0, 13.2	NA	NA
197	2,2',3,3',4,4',6,6'-八氯联苯 2,2',3,3',4,4',6,6'-Octachloro	33091-17-7	NA	25.7	NA	NA
198	2,2',3,3',4,5,5',6-八氯联苯 2,2',3,3',4,5,5',6-Octachloro	68194-17-2	NA	1.4, 15.6	NA	NA
199	2,2',3,3',4,5,5',6'-八氯联苯 2,2',3,3',4,5,5',6'-Octachloro	52663-75-9	NA	1.0, 23.0	NA	NA
200	2,2',3,3',4,5,6,6'-八氯联苯 2,2',3,3',4,5,6,6'-Octachloro	52663-73-7	NA	24.4	NA	NA

Table E.2. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)	辛醇-水分配系数 log K _{ow} ^b
201	2,2',3,3',4,5',6,6'-八氯联苯 2,2',3,3',4,5',6,6'-Octachloro	40186-71-8	NA	1.7 - 95.8	NA	NA
202	2,2',3,3',5,5',6,6'-八氯联苯 2,2',3,3',5,5',6,6'-Octachloro	2136-99-4	NA	1.8, 22.6	1.82 - 75.79	7.10 - 9.77
203	2,2',3,4,4',5,5',6-八氯联苯 2,2',3,4,4',5,5',6-Octachloro	52663-76-0	NA	14.2	NA	NA
204	2,2',3,4,4',5,6,6'-八氯联苯 2,2',3,4,4',5,6,6'-Octachloro	74472-52-9	NA	34.9	NA	NA
205	2,3,3',4,4',5,5',6-八氯联苯 2,3,3',4,4',5,5',6-Octachloro	74472-53-0	NA	8.85	NA	NA
206	2,2',3,3',4,4',5,5',6-九氯联苯 2,2',3,3',4,4',5,5',6-Nonachloro	40186-72-9	NA	8.85	27.66	7.20 - 10.44
207	2,2',3,3',4,4',5,6,6'-九氯联苯 2,2',3,3',4,4',5,6,6'-Nonachloro	52663-79-3	NA	17.1	35.97	7.52 - 7.94
208	2,2',3,3',4,5,5',6,6'-九氯联苯 2,2',3,3',4,5,5',6,6'-Nonachloro	52663-77-1	NA	16.9	32.53	7.60 - 10.45
209	2,2',3,3',4,4',5,5',6,6'-九氯联苯 2,2',3,3',4,4',5,5',6,6'- Decachloro	2051-24-3	NA	11.4	12.46 - 100	7.85 - 11.20

^aSander (1999)^bMackay et al. (1992a and b, 1993, 1995)^cChemical Abstract Service numbers from Erickson (1997)^dBrunner et al. (1990); Dunnivant et al. (1992); Bamford et al. (2000)^eNA, not available

Table E.3. Range of reported values of H and log K_{ow} for dioxins at 293-298 K.

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
1	二苯并-对-二噁英 Dibenzo- <i>p</i> -dioxin	262-23-4	NA ^c	12.29, 12.39	3.40 - 4.70
2	氯二苯并-对-二噁英 1-Chlorodibenzo- <i>p</i> -dioxin	39227-53-7	NA	8.38	4.20 - 5.74
3	2-氯二苯并-对-二噁英 2-Chlorodibenzo- <i>p</i> -dioxin	39227-54-8	NA	14.82	4.20 - 5.71
4	2,3-二氯二苯并-对-二噁英 2,3-Dichlorodibenzo- <i>p</i> -dioxin	29446-15-9	NA	6.61	4.70 - 6.23
5	2,7-二氯二苯并-对-二噁英 2,7-Dichlorodibenzo- <i>p</i> -dioxin	33857-26-0	6.0, 8.4	8.11	4.70 - 6.72
6	2,8-二氯恶噁 2,8-Dichlorodibenzo- <i>p</i> -dioxin	38964-22-6	3.6, 3.9	2.13	4.70 - 5.60
7	1,2,4-三氯二苯并-对-二恶英 1,2,4-Trichlorodibenzo- <i>p</i> -dioxin	39227-58-2	NA	3.84	5.10 - 7.77
8	1,2,4-三氯二苯并-对-二恶英 1,2,3,4-Tetrachlorodibenzo- <i>p</i> -dioxin	30756-58-8	2.0, 3.8	3.77	5.50 - 8.97
9	1,2,3,7-四氯二苯并[1,4]二恶英 1,2,3,7-Tetrachlorodibenzo- <i>p</i> -dioxin	67028-18-6	NA	0.77	5.50 - 8.81
10	1,2,3,4-四氯二苯并-对-二恶英 1,3,6,8-Tetrachlorodibenzo- <i>p</i> -dioxin	30746-58-8	NA	0.71, 6.90	5.50 - 9.43
11	2,3,7,8-四氯二苯并对-二噁英 2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	1746-01-6	NA	0.0021-10.34	5.38 - 8.93
12	1,2,3,4,7-五氯二苯并-对-二恶英 1,2,3,4,7-Pentachlorodibenzo- <i>p</i> -dioxin	39227-61-7	NA	0.264	6.60 - 10.05
13	1,2,3,4,7,8-六氯二苯并-对-二恶英 1,2,3,4,7,8-Hexachlorodibenzo- <i>p</i> -dioxin	39227-26-8	NA	4.52	7.30 - 10.89
14	1,2,3,4,6,7,8-七氯二苯并-对-二恶英 1,2,3,4,6,7,8-Heptachlorodibenzo- <i>p</i> - dioxin	35822-46-9	NA	0.133	7.92 - 11.98
15	1,2,3,4,6,7,8,9-八氯二苯并-对-二恶英 Octachlorodibenzo- <i>p</i> -dioxin	3268-87-9	NA	0.683	7.33 - 13.08

^aSander (1999).

^bMackay et al. (1992a and b, 1993, 1995)

^cNA, not available

Table E.4. Range of reported values of H and log K_{ow} for dibenzofurans at 293-298 K.

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)
1	二苯并呋喃 Dibenzofuran	132-64-9	NA ^c	3.86 - 4.57
2	2,8-二氯二苯并呋喃 2,8-Dichlorodibenzofuran	5409-83-6	NA	4.91 - 6.16
3	2,4,7,8-四氯二苯并呋喃 2,3,7,8-Tetrachlorodibenzofuran	51207-31-9	1.50, 1.70	5.82 - 7.70
4	2,4,7,8-四氯二苯并呋喃 2,3,4,7,8-Pentachlorodibenzofuran	51207-31-4	NA	6.92 - 7.82
5	1,2,3,4,7,8-六氯二苯并呋喃 1,2,3,4,7,8-Hexachlorodibenzofuran	70658-26-9	NA	7.70
6	1,2,3,6,7,8-六氯二苯并呋喃 1,2,3,6,7,8-Hexachlorodibenzofuran	57117-44-9	NA	NA
7	1,2,3,4,6,7,8-七氯二苯并呋喃 1,2,3,4,6,7,8- Heptachlorodibenzofuran	67462-39-4	NA	7.90 - 9.25
8	1,2,3,6,7,8,9-七氯二苯并呋喃 1,2,3,4,7,8,9-Heptachlorodibenzofuran	55673-89-7	NA	6.90
9	八氯二苯并呋喃 Octachlorodibenzofuran	39001-02-0	0.10	7.05 - 13.93

^bMackay et al. (1992a and b, 1993, 1995)

^cNA, not available

Table E.5. Range of reported values of H and log K_{ow} for polycyclic organic matter (POM) at 293-298 K.

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
1	二氢化茚 Indan	496-11-7	NA ^c	NA	3.30 - 3.57
2	萘 Naphthalene	91-20-3	42 - 130	29.2 - 123.95	3.01 - 4.70
3	1-甲基萘 1-Methylnaphthalene	90-12-0	26 - 44	16.0 - 45.0	3.86 - 5.08
4	2-甲基萘 2-Methylnaphthalene	91-57-6	41 - 2.0 x 10 ⁴	20.265 - 58.75	3.70 - 5.08
5	1,2-二甲基萘 1,2-Dimethylnaphthalene	573-98-8	NA	NA	NA
6	1,3-二甲基萘 1,3-Dimethylnaphthalene	575-41-7	72	NA	4.36 - 4.55
7	1,4-二甲基萘 1,4-Dimethylnaphthalene	571-58-4	51	NA	4.36 - 4.44
8	1,5-二甲基萘 1,5-Dimethylnaphthalene	571-61-9	63	35.5 - 36.3	4.35 - 4.44
9	2,3-二甲基萘 2,3-Dimethylnaphthalene	581-40-8	60	38.92 - 92.16	4.18 - 4.44
10	2,6-二甲基萘 2,6-Dimethylnaphthalene	581-40-2	120	6.53	4.31 - 4.44
11	1-乙基萘 1-Ethylnaphthalene	1127-76-0	38	14.8 - 36.47	3.87 - 4.42
12	2-乙基萘 2-Ethylnaphthalene	939-27-5	63 , 84	82.2	4.38 - 4.43
13	三甲基萘 1,4,5-Trimethylnaphthalene	2131-41-1	NA	23.50	4.79 - 4.94
14	联苯 Biphenyl	92-52-4	28 - 84	NA	NA
15	4-甲基联苯 4-Methylbiphenyl	644-08-6	NA	NA	4.63 - 4.91
16	4,4'-二甲基联苯 4,4'-Dimethylbiphenyl	613-33-2	NA	NA	5.09 - 5.40
17	二苯甲烷 Diphenylmethane	101-81-5	NA	NA	4.14 - 4.36
18	1,2-二苯乙烷 Bibenzyl	103-29-7	NA	NA	3.67 - 4.82

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
19	反式-1,2 二苯乙烯 <i>trans</i> -Stilbene	103-30-0	NA	NA	4.53 - 4.81
20	萵 Acenaphthene	83-32-9	7.8 - 160	6.45 - 24.79	3.32 - 4.49
21	萵烯 Acenaphthylene	208-96-8	NA	8.40 - 146.9	3.55 - 4.08
22	芴 Fluorene	86-73-7	8.4 - 12	1.90 - 33.4	3.91 - 4.47
23	1-甲基芴 1-Methylfluorene	1730-37-6	NA	NA	4.63 - 4.97
24	菲 Phenanthrene	85-01-8	2.6 - 11	2.06 - 22.9	3.60 - 5.92
25	1-甲基菲 1-Methylphenanthrene	832-69-6	NA	NA	5.14

Table E.5. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
26	蒽 Anthracene	120-12-7	1.8 - 72	1.80 - 110	3.45 - 4.79
27	9-甲基蒽 9-Methylanthracene	779-02-2	NA	NA	4.61 - 5.65
28	2-甲基蒽 2-Methylanthracene	613-12-7	NA	NA	5.14 - 5.15
29	9,10-二甲基蒽 9,10-Dimethylanthracene	781-43-1	NA	NA	5.25 - 5.67
30	芘 Pyrene	129-00-0	1.1, 1.2	0.517 - 12.4	4.45 - 6.70
31	荧蒽 Fluoranthene	206-44-0	0.92, 220	0.659 - 220	4.70 - 6.50
32	1,2-苯并芴 Benzo[a]fluorene	238-84-6	NA	NA	5.32 - 5.75
33	四甲基茚 Benzo[b]fluorene	243-17-4	NA	NA	5.27 - 5.75
34	蒽 Chrysene	218-01-9	NA	0.065 - 0.45	5.01 - 7.10
35	9,10-苯并菲 Triphenylene	217-59-4	NA	NA	5.20 - 7.10
36	对三联苯 <i>p</i> -Terphenyl	92-94-4	NA	NA	5.88 - 6.03
37	并四苯 Naphthacene	92-24-0	NA	NA	5.26 - 6.02
38	苯并[a]蒽 Benz[a]anthracene	56-55-3	NA	0.1013 - 5.17	5.48 - 7.50
39	苯并[b]荧蒽 Benzo[b]fluoranthene	205-99-2	6.8×10^{-2}	0.051 - 3.55	5.78 - 6.61
40	苯并[j]荧蒽 Benzo[j]fluoranthene	205-82-3	NA	NA	6.40 - 6.44
41	苯并[k]荧蒽 Benzo[k]fluoranthene	207-08-9	6.0×10^{-2}	0.016 - 7.50	5.86 - 7.20
42	苯并[a]芘 Benzo[a]pyrene	50-32-8	4.6×10^{-2} , 630	0.034 - 0.810	5.78 - 8.50

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
43	苯并[e]芘 Benzo[e]pyrene	192-97-2	NA	NA	6.44 - 7.40
44	芘 Perylene	198-55-0	NA	0.440	4.80 - 6.53
45	7,12-二甲基苯并[a]蒽 7,12-Dimethylbenz[a] anthracene	57-97-6	NA	NA	5.80 - 6.95
46	9,10-二甲基苯并[a]蒽 9,10-Dimethylbenz[a] anthracene	56-56-4	NA	NA	6.93
47	3-甲基胆蒽 3-Methylcholanthrene	56-49-5	NA	NA	6.42 - 7.11
48	苯并[ghi]芘 Benzo[ghi]perylene	191-24-2	3.4 x 10 ⁻²	0.0146 - 0.709	5.95 - 7.60
49	并五苯 Pentacene	135-48-8	NA	NA	7.19
50	1,2:3,4-二苯并蒽 Dibenz[a,c]anthracene	215-58-7	NA	NA	NA
51	二苯并[a,h]蒽 Dibenz[a,h]anthracene	53-70-3	NA	0.0074, 0.0076	5.80 - 7.19
52	二苯并[a,i]蒽 Dibenz[a,i]anthracene	58-70-3	NA	NA	7.11 - 7.19
53	蔻 Coronene	191-07-1	NA	NA	5.40 - 8.20

^aSander (1999).

^bMackay et al. (1992a and b, 1993, 1995)

^cNA, not available

Table E.6. Range of reported values of H and log K_{ow} for coke oven emissions at 293-298 K – monoaromatic and phenolic compounds.

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
1	乙苯 Ethylbenzene	100-41-4	600 - 920	653 - 1001	2.68 - 3.43
2	1,2,3-三甲苯 1,2,3-Trimethylbenzene	526-73-8	330, 380	323 - 441	3.31 - 3.81
3	偏三甲苯 1,2,4-Trimethylbenzene	95-63-6	560 - 680	385 - 1242	3.31 - 3.82
4	1,3,5-三甲苯 1,3,5-Trimethylbenzene	108-67-8	600 - 840	600 - 1459	3.41 - 4.32
5	丙基苯 <i>n</i> -Propylbenzene	103-65-1	720 - 1.1 x 10 ³	700 - 1175	3.42 - 3.90
6	异丙苯 Isopropylbenzene	98-82-8	130 - 1.5 x 10 ³	909 - 1521	3.23 - 3.66
7	邻乙基甲苯 1-Ethyl-2-methylbenzene	611-14-3	420, 440	427 - 565	3.53 - 3.63
8	3-乙基甲苯 1-Ethyl-3-methylbenzene	620-14-4	NA ^c	NA	NA
9	4-乙基甲苯 1-Ethyl-4-methylbenzene	622-96-8	510	498	3.63
10	4-异丙基甲苯 1-Isopropyl-4-methylbenzene	99-87-6	780	800	3.45 - 4.14
11	丁苯 <i>n</i> -Butylbenzene	104-51-8	1.3 x 10 ³	1300 - 1692	3.18 - 4.60
12	异丁基苯 Isobutylbenzene	538-93-2	3.3 x 10 ³	1160 - 3300	4.01
13	仲丁基苯 <i>sec</i> -Butylbenzene	135-98-8	1.2 x 10 ³ , 1.4 x 10 ³	1400 - 1838	NA
14	叔丁基苯 <i>tert</i> -Butylbenzene	98-06-6	1.2 x 10 ³	1200 - 1300	4.01 - 4.11
15	1,2,3,4-四甲基苯 1,2,3,4- Tetramethylbenzene	48-23-3	NA	NA	3.84 - 5.02
16	1,2,3,5-四甲基苯 1,2,3,5-Tetramethylbenzene	527-53-7	NA	NA	4.04 - 5.02

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
17	1,2,4,5-四甲基苯 1,2,4,5-Tetramethylbenzene	95-93-2	2.5 x 10 ³ , 2.6 x 10 ³	2540, 2552	2.80 - 4.24
18	戊基苯 <i>n</i> -Pentylbenzene	538-68-1	600, 1.7 x 10 ³	600, 617	4.56 - 4.90
19	五甲基苯 Pentamethylbenzene	538-61-1	NA	NA	4.56 - 4.63
20	己基苯 <i>n</i> -Hexylbenzene	1077-16-3	2.2 x 10 ³	1977	5.24 - 5.52
21	六甲基苯 Hexamethylbenzene	87-85-4	NA	NA	4.02 - 5.16
22	2,3-二甲苯酚 2,3-Dimethylphenol	526-75-0	NA	NA	NA
23	2,4-二甲苯基酚 2,4-Dimethylphenol	105-67-9	0.25, 530	0.0638 - 1.722	1.99 - 3.20
24	2,4 -二甲苯基酚 2,5-Dimethylphenol	105-67-9	NA	NA	NA
25	2,6 -二甲苯基酚 2,6-Dimethylphenol	576-26-1	NA	0.0193 - 0.684	2.07 - 2.51

Table E.6. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
26	3,4-二甲基苯酚 3,4-Dimethylphenol	95-65-8	NA	0.00942 - 0.02120	2.23 - 2.47
27	3,5-二甲基苯酚 3,5-Dimethylphenol	108-68-9	NA	NA	NA
28	2,3,5-三甲基苯酚 2,3,5-Trimethylphenol	697-82-5	NA	0.404	3.06
29	2,3,6-三甲基苯酚 2,3,6-Trimethylphenol	2416-94-6	NA	NA	NA
30	2,4,5-三甲酚 2,4,5-Trimethylphenol	496-78-6	NA	NA	NA
31	2,4,6-三甲酚 2,4,6-Trimethylphenol	527-60-6	NA	0.2512	2.73
32	3,4,5-三甲苯酚 3,4,5-Trimethylphenol	527-54-8	NA	NA	NA
33	3-乙基-5-甲基苯酚 3-Methyl-5-ethylphenol	NA	NA	NA	NA
34	邻乙苯酚 2-Ethylphenol	90-00-6	NA	0.174	2.46 - 2.64
35	3-乙基苯酚 3-Ethylphenol	620-17-7	NA	NA	NA
36	4-乙基苯酚 4-Ethylphenol	123-07-9	NA	0.132	2.12 - 2.81
37	2-正丙基苯酚 2-Propylphenol	644-35-0	NA	NA	NA
38	4-丙基苯酚 4- <i>n</i> -Propylphenol	645-56-7	NA	NA	NA
39	2-异丙基苯酚 2-Isopropylphenol	88-69-7	NA	NA	NA
40	对异丙基苯酚 4-Isopropylphenol	99-89-8	NA	NA	NA
41	4-丁基苯酚 4- <i>n</i> -Butylphenol	1638-22-8	NA	NA	NA
42	2-仲丁基苯酚 2- <i>sec</i> -Butylphenol	89-72-5	NA	NA	NA

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
43	邻叔丁基苯酚 2- <i>tert</i> -Butylphenol	88-18-6	NA	NA	NA
44	3-叔丁基苯酚 3- <i>tert</i> -Butylphenol	585-34-2	NA	NA	NA
45	对仲丁基苯酚 4- <i>sec</i> -Butylphenol	99-71-8	NA	NA	NA
46	4-叔丁基苯酚 4- <i>tert</i> -Butylphenol	98-54-4	0.11	0.113 - 3.750	2.94 - 3.41
47	5-叔丁基-2-甲基苯酚 2-Methyl-5- <i>tert</i> -Butylphenol	NA	NA	NA	NA
48	2,6-二叔丁基苯酚 2,6-Di- <i>sec</i> -Butylphenol	128-39-2	NA	NA	NA
49	3,5-二叔丁基苯酚 3,5-Di- <i>tert</i> -Butylphenol	1138-52-9	NA	NA	NA
50	2,6-二叔丁基-4-甲基苯酚 2,6-Di- <i>t</i> -butyl-4-Methylphenol	128-37-0	NA	NA	NA

Table E.6. (Cont.).

No.	Chemical	CAS No.	亨利定律常数 Henry's Law constant, H ^a (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^d (Pa m ³ mol ⁻¹)	亨利定律常数 Henry's Law constant, H ^b (Pa m ³ mol ⁻¹)
51	3-戊基苯酚 3-Pentylphenol	NA	NA	NA	NA
52	4-己基苯酚 4-Hexylphenol	2446-69-7	NA	NA	NA
53	2-庚基苯酚 2-Heptylphenol	NA	NA	NA	NA
54	4-庚基苯酚 4-Heptylphenol	1987-50-4	NA	NA	NA
55	4-辛基酚 4-Octylphenol	1806-26-4	NA	0.4916	3.70, 4.12
56	对特辛基苯酚 4- <i>tert</i> -Octylphenol	140-66-9	NA	NA	NA
57	对壬基酚 4-Nonylphenol	104-40-5	NA	1.5705	4.10 - 6.36
58	1-萘酚 1-Naphthol	90-15-3	NA	0.49	2.28 - 3.13
59	2-萘酚 2-Naphthol	135-19-3	NA	0.280	2.01 - 3.46
60	邻苯基苯酚 2-Phenylphenol	90-43-7	NA	NA	3.09 - 3.36
61	间羟基联苯 3-Phenylphenol	588-51-8	NA	NA	NA
62	对羟基联苯 4-Phenylphenol	92-69-3	NA	NA	2.88 - 3.63
63	2-烯丙基酚 2-Allylphenol	1745-81-9	NA	NA	NA

^aSander (1999).

^bMackay et al. (1992a and b, 1993, 1995)

^cNA, not available