

APPENDIX A. ENVIRONMENTAL CHEMISTRY

The tables in this appendix are discussed in Chapter 2. References listed at the end of each table are included in the reference list at the end of Chapter 2. Following are the tables included in this Appendix:

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Table A-1. P-Chem Properties for the Dioxin, Furan, and PCB Congeners

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
Tetrachlorodibenzo-p-dioxins (MW = 321.98)												
1,2,3,4-TCDD 30746-58-8	3.88E-04- 6.30E-04 [5.50E-04]	25 [25]	5,38,46,51,53 [53]	1.81E-08- 4.80E-08 [4.80E-08]	25 [25]	9,33,53 [9,53]	1.99E-05- (3.70E-05) [1.99E-05]	5,51,53 [51]	(5.50)- (8.97) [6.60]	5,7,8,10, 26,29,53 [53]		
1,2,3,6-TCDD 71669-25-5									6.86	10		
1,2,3,7-TCDD 67028-18-6	2.80E-04- 7.30E-04 [4.20E-04]	20-26 [20]	6,53 [6,53]	(7.50E-09)- (5.3E-08) [7.50E-09]	25 [25]	9,21,52,5 3 [21,53]	(7.57E-06)	9,53	(5.50)- (8.81) [6.90]	5,7,8,10, 26,53 [53]	4.26- 6.55	45,53
1,2,3,8-TCDD 53555-02-5									6.48	10		
1,2,3,9-TCDD 71669-26-6									6.39	10		
1,2,4,6-TCDD 71669-27-7									6.10	10		
1,2,4,7-TCDD 71669-28-8									6.25	10		
1,2,4,8-TCDD 71669-29-9									6.25	10		
1,2,4,9-TCDD 71665-99-1									6.10	10		
1,2,6,7-TCDD 40581-90-6												
1,2,6,8-TCDD 67323-56-2									6.43	10		
1,2,6,9-TCDD 40581-91-7												

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,7,8-TCDD 34816-53-0									6.38	10		
1,2,7,9-TCDD 71669-23-3									6.86	10		
1,2,8,9-TCDD 62470-54-6												
1,3,6,8-TCDD 33423-92-6	1.68E-04- (6.0E-04) [3.2E-04]	20-25 [20]	6,7,38,53 [7,53]	(5.25E-09)- 4.03E-06 [5.25E-09]	20-25 [25]	7,9,53 [9,53]	(5.92E-06)- 6.81E-05 [6.95E-06]	5,7,53 [53]	(5.5)-(9.43) [7.10]	5,7,8,10, 26,53 [5,53]	2.05- (6.74)	53
1,3,6,9-TCDD 71669-24-4									6.25	10		
1,3,7,8-TCDD 50585-46-1				(6.3E-09)	25	9			6.30	10		
1,3,7,9-TCDD 62470-53-5									6.39-7.06 [6.39]	8,10 [10]		
1,4,6,9-TCDD 40581-93-9									6.38	10		
1,4,7,8-TCDD 40581-94-0									6.39	10		
2,3,7,8-TCDD 1746-01-6	7.91E-06- 4.83E-04 [1.93E-05]	17-25 [25]	1,2,4,5,27, 36,50,53 [4,53]	7.40E-10- 3.38E-08 [1.50E-09]	25 [25]	2,3,5,9,3 4,53 [9,53]	(2.07E-08)- (1.02E-04) [3.29E-05]	2,3,5,53 [53]	5.38-8.93 [6.80]	2,4,5,8,10, 50,53 [53]	3.06- 8.50 [6.4- 6.66]	32,47,48, 49,50,53,57 [50,57]
Congener Group Average	(3.3E-04)	25	20	(1.4E-08)	25	20	(1.7E-05)	20	(6.5)	20		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm·m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
Pentachlorodibenzo-p-dioxins (MW = 356.42)												
1,2,3,4,6-PeCDD 67028-19-7									6.30	10		
1,2,3,4,7-PeCDD 39227-61-7	9.55E-05- 8.16E-03 [1.18E-04]	20-26 [20]	5,6,38,53 [6,53]	(6.60E-10)- 7.5E-09 [6.60E-10]	25 [25]	5,9,53 [9,53]	(2.63E-06)	5,53	6.60- (10.05) [7.40]	5,7,8,10, 26,53 [53]	4.85- 6.38	45,53
1,2,3,6,7-PeCDD 71925-15-0									6.74	10		
1,2,3,6,8-PeCDD 71925-16-1									6.53	10		
1,2,3,6,9-PeCDD 82291-34-7									6.24	10		
1,2,3,7,8-PeCDD 40321-76-4				(4.4E-10)- 9.48E-10 [4.40E-10]	25 [25]	9,33 [9]			6.64	10		
1,2,3,7,9-PeCDD 71925-17-2									6.40	10		
1,2,3,8,9-PeCDD 71925-18-3												
1,2,4,6,7-PeCDD 82291-35-8												
1,2,4,6,8-PeCDD 71998-76-0												
1,2,4,6,9-PeCDD 82291-36-9									6.60	10		
1,2,4,7,8-PeCDD 58802-08-7				(5.8E-10)	25	9			6.20	10		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,4,7,9-PeCDD 82291-37-0												
1,2,4,8,9-PeCDD 82291-38-1												
Congener Group Average	(1.18E-04)	20	20	(5.6E-10)	25	20	(2.6E-06)	20	(6.6)	20		
Hexachlorodibenzo-p-dioxins (MW = 390.87)												
1,2,3,4,6,7- HxCDD 58200-66-1												
1,2,3,4,6,8- HxCDD 58200-67-2									6.85	10		
1,2,3,4,6,9- HxCDD 58200-68-3												
1,2,3,4,7,8- HxCDD 39227-28-6	4.00E-06- 6.44E-06 [4.42E-06]	21-26 [25]	5,6,53 [6,53]	(3.8E-11)- 1.01E-10 [3.8E-11]	25 [25]	5,9,33, 53 [9,53]	(1.07E-05)- (4.46E-05) [1.07E-05]	5,19,53 [53]	7.79-10.44 [7.80]	7,8,26,53 [53]	5.02- (7.10)	45,53
1,2,3,6,7,8- HxCDD 57653-85-7				(3.6E-11)	25	9						
1,2,3,6,7,9- HxCDD 64461-98-9									7.59	10		
1,2,3,6,8,9- HxCDD 58200-69-4									7.59	10		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm·m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,3,7,8,9- HxCDD 19408-74-3				(4.9E-11)	25	9						
1,2,4,6,7,9- HxCDD 39227-62-8				(5.1E-11)	25	9			6.85	10		
1,2,4,6,8,9- HxCDD 58802-09-8									6.85	10		
Congener Group Average	(4.4E-06)	25	20	(4.4E-11)	25	20	(1.1E-05)	20	(7.3)	20		
Heptachlorodibenzo-p-dioxins (MW = 425.31)												
1,2,3,4,6,7,8- HpCDD 35822-46-9	2.3E-06- 2.56E-06 [2.4E-06]	20-26 [20]	5,6,53 [6,53]	(5.6E-12)- (2.40E-10) [5.6E-12]	25 [25]	9,33,53 [9,53]	(1.31E-06)- (1.26E-05) [1.26E-05]	5,53 [53]	7.92- (11.98) [8.00]	7,8,10,26, 53 [53]	5.47- (7.80)	53
1,2,3,4,6,7,9- HpCDD 58200-70-7												
Congener Group Average	(2.4E-06)	20	20	(5.6E-12)	25	20	(1.3E-05)	20	(8.0)	20		
Octachlorodibenzo-p-dioxin (MW = 460.76)												
1,2,3,4,6,7,8,9- OCDD 3268-87-9	7.4E-08- 7.36E-06 [7.4E-08]	20-25 [25]	5,6,7,53 [5,53]	(8.25E-13)- 6.54E-08 [8.25E-13]	20-25	7,9,33, 53 [9,53]	(6.75E-06)	5,53	(7.5)-(13) [8.20]	5,7,8,26, 29,53 [5,53]	5.92- (7.90)	53
Tetrachlorodibenzofurans (MW = 305.98)												
1,2,3,4-TCDF 30402-14-3				(3.1E-08)	25	21			6.17	10		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,3,6-TCDF 83704-21-6									6.15	10		
1,2,3,7-TCDF 83704-22-7				(3.2E-08)	25	21						
1,2,3,8-TCDF 62615-08-1				(2.1E-08)	25	21			6.15	10		
1,2,3,9-TCDF 83704-23-8									6.06	10		
1,2,4,6-TCDF 71998-73-7												
1,2,4,7-TCDF 83719-40-8												
1,2,4,8-TCDF 64126-87-0				(2.2E-08)	25	21			6.31	10		
1,2,4,9-TCDF 83704-24-9												
1,2,6,7-TCDF 83704-25-0				(2.0E-08)	25	21			6.25	10		
1,2,6,8-TCDF 83710-07-0												
1,2,6,9-TCDF 70648-18-9												
1,2,7,8-TCDF 58802-20-3				(1.8E-08)	25	21			6.23	10		
1,2,7,9-TCDF 83704-26-1				(2.5E-08)	25	21			6.25	10		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm·m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,8,9-TCDF 70648-22-5												
1,3,4,6-TCDF 83704-27-2									6.31	10		
1,3,4,7-TCDF 70648-16-7									6.23	10		
1,3,4,8-TCDF 92341-04-3									6.13	10		
1,3,4,9-TCDF 83704-28-3									5.89	10		
1,3,6,7-TCDF 57117-36-9				(2.8E-08)	25	21						
1,3,6,8-TCDF 71998-72-6				(2.7E-08)	25	21			6.37	10		
1,3,6,9-TCDF 83690-98-6												
1,3,7,8-TCDF 57117-35-8									6.34	10		
1,3,7,9-TCDF 64560-17-4				(1.9E-08)	25	21			6.34	10		
1,4,6,7-TCDF 66794-59-0				(2.6E-08)	25	21			6.15	10		
1,4,6,8-TCDF 82911-58-8												
1,4,6,9-TCDF 70648-19-0									5.60	10		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,4,7,8-TCDF 83704-29-4												
1,6,7,8-TCDF 83704-33-0									6.17	10		
2,3,4,6-TCDF 83704-30-7				(4.0E-08)	25	21			6.11	10		
2,3,4,7-TCDF 83704-31-8				(2.9E-08)	25	21			6.06	10		
2,3,4,8-TCDF 83704-32-9				(2.8E-08)	25	21						
2,3,6,7-TCDF 57117-39-2				(2.1E-08)	25	21			6.31	10		
2,3,6,8-TCDF 57117-37-0				(2.0E-08)	25	21			6.73	10		
2,3,7,8-TCDF 51207-31-9	4.19E-04	22.7	11	8.96E-09- (1.5E-08) [1.5E-08]	25 [25]	21,33,53 [21,53]	(1.44E-05)- (1.48E-05) [1.44E-05]	53,54 [53]	5.82-6.53 [6.1]	8,10,53 [53]	(5.20)- (7.50)	53
2,4,6,7-TCDF 57117-38-1				(3.3E-08)	25	21			6.25	10		
2,4,6,8-TCDF 58802-19-0				(2.0E-08)	25	21			6.17	10		
3,4,6,7-TCDF 57117-40-5												
Congener Group Average	(4.2E-04)	22.7	20	(2.5E-08)	25	20	(1.4E-05)	20	(6.2)	20		
Pentachlorodibenzofurans (MW = 340.42)												

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm·m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,3,4,6-PeCDF 83704-47-6				(2.7E-09)	25	21						
1,2,3,4,7-PeCDF 83704-48-7									6.53	10		
1,2,3,4,8-PeCDF 67517-48-0				(3.6E-09)	25	21			6.79	10		
1,2,3,4,9-PeCDF 83704-49-8												
1,2,3,6,7-PeCDF 57117-42-7				(2.2E-09)	25	21			6.26	10		
1,2,3,6,8-PeCDF 83704-51-2									6.33	10		
1,2,3,6,9-PeCDF 83704-52-3												
1,2,3,7,8-PeCDF 57117-41-6				(1.7E-09)- 2.72E-09 [1.7E-09]	25	21,33 [21]			6.79	10		
1,2,3,7,9-PeCDF 83704-53-4												
1,2,3,8,9-PeCDF 83704-54-5												
1,2,4,6,7-PeCDF 83704-50-1				(3.5E-09)	25	21			6.27	10		
1,2,4,6,8-PeCDF 69698-57-3				(2.3E-09)	25	21			6.34	10		
1,2,4,6,9-PeCDF 70648-24-7									6.59	10		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,4,7,8-PeCDF 58802-15-6				(1.5E-09)	25	21			6.26	10		
1,2,4,7,9-PeCDF 71998-74-8				(2.6E-09)	25	21			6.19	10		
1,2,4,8,9-PeCDF 70648-23-6												
1,2,6,7,8-PeCDF 69433-00-7				(1.9E-09)	25	21			6.42	10		
1,2,6,7,9-PeCDF 70872-82-1									6.51	10		
1,3,4,6,7-PeCDF 83704-36-3				(2.7E-09)	25	21			6.19	10		
1,3,4,6,8-PeCDF 83704-55-6									6.24	10		
1,3,4,6,9-PeCDF 70648-15-6									6.34	10		
1,3,4,7,8-PeCDF 58802-16-7				(4.3E-09)	25	21						
1,3,4,7,9-PeCDF 70648-20-3									6.33	10		
1,3,6,7,8-PeCDF 70648-21-4												
1,4,6,7,8-PeCDF 83704-35-2									6.53	10		
2,3,4,6,7-PeCDF 57117-43-8				(2.4E-09)	25	21			6.47	10		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm·m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
2,3,4,6,8-PeCDF 67481-22-5				(1.9E-09)	25	21			6.59	10		
2,3,4,7,8-PeCDF 57117-31-4	2.36E-04	22.7	11	(2.63E-09)- 3.29E-09 [2.63E-09]	25 [25]	21,33 [53]	(4.98E-06)	53	6.92-(7.82) [6.5]	10,53 [53]	5.59- (7.40)	53
Congener Group Average	(2.4E-04)	22.7	20	(2.7E-09)	25	20	(5.0E-06)	20	(6.4)	20		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
Hexachlorodibenzofurans (MW = 374.87)												
1,2,3,4,6,7- HxCDF 79060-60-9				(2.4E-10)	25	21						
1,2,3,4,6,8- HxCDF 69698-60-8				(2.2E-10)	25	21						
1,2,3,4,6,9- HxCDF 91538-83-9				(4.1E-10)	25	21						
1,2,3,4,7,8- HxCDF 70648-26-9	8.25E-06	22.7	11	(2.4E-10)- (6.7E-10) [2.4E-10]	25 [25]	21,52,53 [21,53]	(1.43E-05)	19	(7.0)	53	(7.40)	53
1,2,3,4,7,9- HxCDF 91538-84-0				(2.8E-10)	25	21						
1,2,3,4,8,9- HxCDF 92341-07-6												
1,2,3,6,7,8- HxCDF 57117-44-9	1.77E-05	22.7	11	(2.2E-10) - (6.68E-10) [2.2E-10]	25 [25]	21,53 [21,53]	(6.1E-06)- (7.31E-06) [7.31E-06]	19,53 [53]				
1,2,3,6,7,9- HxCDF 92341-06-5												
1,2,3,6,8,9- HxCDF 75198-38-8				(3.4E-10)	25	21						

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm·m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,3,7,8,9- HxCDF 72918-21-9				(1.8E-10)	25	21						
1,2,4,6,7,8- HxCDF 67562-40-7				(2.6E-10)	25	21						
1,2,4,6,7,9- HxCDF 75627-02-0				(5.7E-10)	25	21						
1,2,4,6,8,9- HxCDF 69698-59-5				(1.8E-10)	25	21						
1,3,4,6,7,8- HxCDF 71998-75-9				(2.3E-10)	25	21						
1,3,4,6,7,9- HxCDF 92341-05-4												
2,3,4,6,7,8- HxCDF 60851-34-5				(2.0E-10)	25	21						
Congener Group Average	(1.3E-05)	22.7	20	(2.8E-10)	25	20	(1.1E-05)	20	(7.0)	20		
Heptachlorodibenzofurans (MW = 409.31)												
1,2,3,4,6,7,8- HpCDF 67562-39-4	1.35E-06	22.7	11	(3.5E-11)- 1.33E-10 [3.5E-11]	25 [25]	21,33 [21,53]	(1.41E-05)- (5.3E-05) [1.41E-05]	19,53 [53]	7.92-(9.25) [7.4]	10,53 [53]	6.00- (7.90)	53

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
1,2,3,4,6,7,9- HpCDF 70648-25-8												
1,2,3,4,6,8,9- HpCDF 69698-58-4				(5.8E-11)	25	21						
1,2,3,4,7,8,9- HpCDF 55673-89-7				(4.7E-11)- 1.07E-10 [4.7E-11]	25 [25]	21,33 [21,53]					5.00- (6.70)	53
Congener Group Average	(1.4E-06)	22.7	20	(4.7E-11)	25	20	(1.4E-05)	20	(7.4)	20		
Octachlorodibenzofurans (MW = 444.76)												
1,2,3,4,6,7,8,9- OCDF 39001-02-0	(1.16E-06)	25	11	(3.75E-12)	25	21	(1.88E-06)	19	(7.0)-(13) [8.0]	8,26,29,53 [53]	6.00- (7.40)	53
Tetrachloro-PCB (MW = 291.99)												
3,3',4,4'-TCB 32598-13-3	(5.5E-04)- (1.7E-01) [1.03E-03]	25	12,13,17,28,3 5,38,40,44,56 [56]	1.37E-07- 4.47E-07 [4.47E-07]	25	13,18,56 [56]	1.70E-05- (1.0E-04) [1.70E-05]	13,35,39, 56 [56]	5.62-6.77 [6.5]	8,15,31,55 ,56 [56]	(4.41)- (5.75)	56
3,4,4',5-TCB 70362-60-4 (81)	2.92E-03	25	17	(7.85E-07)	25	18	1.28E-04	41	(6.36)	15		
Pentachloro-PCB (MW = 326.44)												
2,3,3',4,4'-PeCB 32598-14-4	(1.9E-03)- (1.1E-02) [1.90E-03]	25	17,35,37,56 [35]	(8.28E-07)	25	18	(6.0E-05)- (9.93E-05) [9.93E-05]	16,35 [35]	(6.3)-(6.6) [6.0]	15,37,55, 56 [56]		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
2,3,4,4',5-PeCB 74472-37-0	(2.58E-03)- (1.1E-02) [2.58E-03]	20-25 [20]	17,35,37,41 [41]	(4.18E-07)- (1.43E-04) [4.18E-07]	20-25 [20]	18,41 [41]	6.90E-05- (1.4E-04) [6.90E-05]	16,35,41 [41]	(6.3)-(6.65) [6.65]	15,37 [15]		
2,3',4,4',5-PeCB 31508-00-6	(1.59E-03)- (1.1E-02) [1.59E-03]	20-25 [20]	17,35,37,41 [41]	(3.14E-07)- (1.38E-06) [3.14E-07]	20-25 [20]	18,41 [41]	8.50E-05- 4.0E-04 [8.50E-05]	16,35,41, 43 [41]	(6.2)-7.12 [7.12]	15,31,37, 55 [31]	(5.7)	42
3,3',4,4',5-PeCB 57465-28-8	(1.03E-03)	25	17	(2.19E-07)- (3.72E-07) [2.96E-07]	25	18 [18]	(5.4E-05)- (8.2E-05) [5.40E-05]	16,35 [35]	(6.26)- (6.89) [6.89]	15,37 [15]		
2',3,4,4',5-PeCB 65510-44-3	(1.64E-03)	25	17	(7.62E-07)- (9.95E-07) [8.78E-07]	25	18 [18]	(1.74E-04)- (2.62E-04) [1.74E-04]	16,35 [35]	(6.74)	15		
Hexachloro-PCB (MW = 360.88)												
2,3,3',4,4',5- HxCB 38380-08-4	(4.10E-04)- (2.4E-03) [4.10E-04]	20-25 [20]	17,37,41 [41]	(1.47E-07)	25	18	(2.2E-05)- 8.7E-04 [8.70E-04]	16,35,43 [43]	(6.64)- (7.16) [7.16]	14,15,37 [14]		
2,3,3',4,4',5'- HxCB 69782-90-7	(3.61E-04)	25	17	(5.47E-08)- (1.08E-07) [5.47E-08]	25	18	(6.6E-05)- 5.8E-04 [5.80E-04]	16,35,43 [43]	7.18-(7.20) [7.19]	14,15 [14]		
2,3',4,4',5,5'- HxCB 52663-72-6	(3.61E-04)- (2.44E-03) [3.61E-04]	25	17,37 [17]	(1.46E-07)- (1.95E-07) [1.95E-07]	25	18	(1.1E-04)- (1.2E-04) [1.10E-04]	16,35 [35]	(6.64)- (7.27) [7.09]	14,15,37 [14]		
3,3',4,4',5,5'- HxCB 32774-16-6	(3.61E-05)- (2.5E-03) [3.61E-05]	25	17,35,37 [17]	(8.1E-09)- (3.5E-07) [1.81E-07] ^d	25	56	(1.6E-05)- (6.5E-05) [6.52E-05]	16,35,56 [35]	(6.64)-7.46 [7.46]	14,15,37, 56 [14]	(6.60)	56
Heptachloro-PCB (MW = 396.33)												
2,3,3',4,4',5,5'- HpCB 39635-31-9	(4.5E-05)- (5.3E-04) [6.26E-05]	25	17,35,37 [17]	(1.19E-08)- (1.73E-08) [1.31E-08]	25	18	(6.6E-05)	35	(7.0)-(7.71) [7.71]	15,37 [15]		

Table A-1 (continued)

Congener	Water Solubility			Vapor Pressure			Henry's Law Constant		Log K _{ow}		Log K _{oc}	
CAS No.	Value ^{a,c} (mg/l)	Temp. (°C)	Ref.	Value ^{a,b} (mm Hg)	Temp. (°C)	Ref.	Value ^a (atm-m ³ /mol)	Ref.	Value ^a	Ref.	Value ^a	Ref.
2,2',3,3',4,4',5-HpCB 35065-30-6	(1.19E-04)- (5.21E-04) [2.27E-04]	20-25 [20]	17,35,37,41 [41]	(6.46E-09)- 8.60E-09 [6.46E-09]	20-25 [25]	18,41 [41]	(1.50E-05)- (8.73E-05) [1.50E-05]	35,41 [41]	(7.03)- (7.27) [7.27]	15,37,42, 56 [15]	5.5-6.8	42,56
2,2',3,4,4',5,5'-HpCB 35069-29-3	(2.25E-04)- (4.40E-04) [4.40E-04]	20-25 [20]	17,35,37,41 [41]	3.39E-08- (2.72E-07) [2.72E-07]	20-25 [25]	18,41 [41]	(3.20E-05)- (1.07E-04) [3.20E-05]	35,41 [41]	(6.70)- (7.36) [7.36]	15,37,42, 56 [15]	5.1-7.4	42,56

Footnote References

^a Values are presented as they appeared in the referenced article. Values in () are either estimated or are calculated/extrapolated from experimental values.

^b [R] is the ranking of the value from the cited reference.

^c For several PCB congeners, subcooled liquid values were converted to solid values using the melting points presented in this table and the conversion methodology presented in Eitzer and Hites (1988) and Mackay et al. (1992).

^d The selected vapor pressure value for PCB-169 is the midpoint of the range of calculated values.

$$\ln (P_{sc}/P_s) = 6.79 (T_m - T)/T$$

where: P_{sc} = subcooled value

P_s = solid value

T_m = melting point (°K)

T = ambient temperature (°K)

1. Marple et al. (1986a)

2. USEPA (1990)

3. Podoll et al. (1986)

4. Marple et al. (1986b)

5. Shiu et al. (1988)

6. Friesen et al. (1985)

7. Webster et al. (1985)

8. Burkhard and Kuehl (1986)

9. Rordorf (1987)

10. Sijm et al. (1989)

11. Friesen et al. (1990b)

12. Dickhut et al. (1986)

20. Average of all selected and single values within a congener group

21. Rordorf (1989)

22. Dulin et al. (1986)

23. Choudhry and Webster (1987)

24. Choudhry and Webster (1989)

25. Choudhry et al. (1990)

26. Sarna et al. (1984)

27. Adams and Blaine (1986)

28. Mackay et al. (1980)

29. Doucette and Andren (1988a)

30. Orth et al. (1989)

31. Rapaport and Eisenreich (1984)

39. Dunnivant et al. (1988)

40. Opperhuizen et al. (1988)

41. Murphy et al. (1987)

42. EPRI (1990)

43. Murphy et al. (1983)

44. Yalkowsky et al. (1983)

45. Webster et al. (1986)

46. Doucette and Andren (1988b)

47. Walters and Guiseppi-Elie (1988)

48. Jackson et al. (1986)

49. Puri et al. (1989)

50. Marple et al. (1987)

Table A-1 (continued)

13. Dunnivant and Elzerman (1988)	32. Lodge and Cook (1989)	51. Santl et al. (1994)
14. Risby et al. (1990)	33. Eitzer and Hites (1988)	52. Rordorf et al. (1990)
15. Hawker and Connell (1988)	34. Rordorf (1985)	53. Mackay et al. (1992a)
16. Sabljic and Gusten (1989)	35. Dunnivant et al. (1992)	54. Eitzer and Hites (1989)
17. Abramowitz and Yalkowsky (1990)	36. Lodge (1989)	55. Sacan and Inel (1995)
18. Foreman and Bidleman (1985)	37. Patil (1991)	56. Mackay, et al. (1992b)
19. Calculated by the VP/WS ratio technique	38. Nirmalakhandan and Speece (1989)	57. Walters et al. (1989)

Table A-2. Rankings for the P-Chem Property Literature

Reference Number	Ranking ^a					
	Water Solubility	Vapor Pressure	Henry's Constant	Log K _{ow}	Log K _{oc}	Photo Quantum Yield
1	2					
3		2	4			
4				1		
5	2		4	1		
6	2					
7	2	2	2	4		
8				4		
9		2 & 4				
10				1 & 2		
11	2					
12	1					
13	1	4	2			
14				3		
15				2 & 5		
16			5			
17	5					
18		2 & 4				
19			5			
20	5	5	5	5	5	
21		2 & 4				
22						2
23						2
24						2
25						2
26				5		
27	2					

Table A-2 (continued)

Reference Number	Ranking ^a					
	Water Solubility	Vapor Pressure	Henry's Constant	Log K _{ow}	Log K _{oc}	Photo Quantum Yield
1	2					
28	5					
29				5		
30						2
31				4		
32					1	
33		4				
34		4				
35	5		5			
36	2					
37	5			5		
38	5					
39			2			
40	2					
41	2	2	4			
42					4	
43			4			
44	5					
45					2	
46	2					
47					1	
48					1	
49					2	
50	1			1	1	
51	2		2			
52		4				

Table A-2 (continued)

Reference Number	Ranking ^a					
	Water Solubility	Vapor Pressure	Henry's Constant	Log K _{ow}	Log K _{oc}	Photo Quantum Yield
1	2					
54			4			
55				4		
57					1	

Footnote References

^a P-chem properties with two ranks indicates that some of the values for the chemicals in the reference had been verified by another laboratory, and some values have not been verified yet. It also indicates that more than one methodology may have been used in the reference to determine the p-chem property.

1. Marple et al. (1986a)
3. Podoll et al. (1986)
4. Marple et al. (1986b)
5. Shiu et al. (1988)
6. Friesen et al. (1985)
7. Webster et al. (1985)
8. Burkhard and Kuehl (1986)
9. Rordorf (1987)
10. Sijm et al. (1989)
11. Friesen et al. (1990)
12. Dickhut et al. (1986)
13. Dunnivant and Elzerman (1988)
14. Risby et al. (1990)
15. Hawker and Connell (1988)
16. Sabljic and Gunsten (1989)
17. Abramowitz and Yalkowsky (1990)
18. Foreman and Bidleman (1985)
19. Calculated by the VP/WS ratio technique
20. Average of all literature values (measured and calculated) within a congener group.
21. Rordorf (1989)
22. Dulin et al. (1986)
23. Choudhry and Webster (1987)
24. Choudhry and Webster (1989)
25. Choudhry et al. (1990)
26. Sarna et al. (1984)
27. Adams and Blaine (1986)
28. Mackay et al. (1980)
29. Doucette and Andren (1988)
30. Orth et al. (1989)
31. Rapaport and Eisenreich (1984)
32. Lodge and Cook (1989)
33. Eitzer and Hites (1988)
34. Rordorf (1985)
35. Dunnivant et al. (1992)
36. Lodge (1989)
37. Patil (1991)
38. Nirmalakhandan and Speece (1989)
39. Dunnivant et al. (1988)
40. Opperhuizen et al. (1988)
41. Murphy et al. (1987)
42. EPRI (199)
43. Murphy et al. (1983)
44. Yalkowsky et al. (1983)
45. Webster et al. (1986)
46. Doucette and Andren (1988)
47. Walters and Guiseppi-Elie (1988)
48. Jackson et al. (1986)
49. Puri et al. (1989)
50. Marple et al. (1987)
51. Santl et al. (1994)
52. Rordorf et al. (1990)
53. Mackay et al. (1992a)
54. Eitzer and Hites (1989)
55. Sacan and Inel (1995)
56. Mackay et al. (1992b)
57. Walters et al. (1989)