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ENVIRONMENTAL ORGANIC CHEMISTRY



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A Wiley-Interscience Publication

JOHN WILEY & SONS, INC.

New York / Chichester / Brisbane / Toronto / Singapore

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Library of Congress Cataloging in Publication Data:

Schwarzenbach, René P., 1945-

Environmental organic chemistry / by René P. Schwarzenbach, Philip M. Gschwend, Dieter M. Imboden.

p. cm.

"A Wiley-Interscience Publication."

Includes bibliographical references and index.

ISBN 0-471-83941-8 (cloth)

1. Organic compounds—Environmental aspects. 2. Water chemistry.

I. Gschwend, P. M. II. Imboden, Dieter M., 1943- . III. Title.

TD196.073S39 1992

628.1'68—dc20

92-10737

Printed in the United States of America

CONTENTS

PREFACE	ix
1 INTRODUCTION	1
2 AN INTRODUCTION TO ENVIRONMENTAL ORGANIC CHEMICALS	8
2.1 Introduction / 8	
2.2 The Makeup of Organic Compounds / 8	
2.3 Classification, Nomenclature, and Examples of Environmental Organic Chemicals / 30	
3 BACKGROUND THERMODYNAMICS	41
3.1 Introduction / 41	
3.2 Using Thermodynamic Functions to Describe Molecular Energies / 42	
3.3 Using Thermodynamic Functions to Quantify Molecular Change Processes / 50	
3.4 Summary / 55	
4 VAPOR PRESSURE	56
4.1 Introduction / 56	
4.2 Thermodynamic Considerations / 58	
4.3 Molecular Interactions Governing Vapor Pressure / 63	

4.4	Availability of Experimental Vapor Pressure Data and Estimation Methods / 70	
5	SOLUBILITY AND ACTIVITY COEFFICIENT IN WATER	76
5.1	Introduction / 76	
5.2	Thermodynamic Considerations / 77	
5.3	Molecular Interpretation of the Dissolution Process / 82	
5.4	Effect of Temperature and Solution Composition on Aqueous Solubility and Activity Coefficient / 90	
5.5	Dissolution of Organic Compounds in Water from Organic Liquid Mixtures / 104	
5.6	Availability of Solubility Data; Estimation of Aqueous Solubility and Activity Coefficient / 107	
6	AIR-WATER PARTITIONING: THE HENRY'S LAW CONSTANT	109
6.1	Introduction / 109	
6.2	Thermodynamic Considerations: Effects of Concentration, Temperature, Salt, and Cosolutes / 112	
6.3	Experimental Determination of Air-Water Partition Ratios / 116	
6.4	Availability of K_H Data—Estimation Methods / 123	
7	ORGANIC SOLVENT-WATER PARTITIONING: THE OCTANOL-WATER PARTITION CONSTANT	124
7.1	Introduction / 124	
7.2	Thermodynamic Considerations and Molecular Interpretation of Solvent-Water Partitioning / 125	
7.3	The <i>n</i> -Octanol-Water Partition Constant (K_{ow}) of Neutral Organic Compounds / 130	
7.4	Approaches Using Chemical Structure to Relate and Estimate Partition Constants / 134	
7.5	Chemical Structure and Partitioning Behavior—Estimation of K_{ow} from Structural Group Contributions / 142	
8	ORGANIC ACIDS AND BASES: ACIDITY CONSTANT AND PARTITIONING BEHAVIOR	157
8.1	Introduction—Acidity Constant / 157	
8.2	Chemical Structure and Acidity Constant / 166	
8.3	Availability of Experimental pK_a Values and pK_a Estimation Methods / 170	
8.4	Comments on Aqueous Solubility and Partitioning Behavior of Organic Acids and Bases / 178	

9	DIFFUSION	182
9.1	The Gradient-Flux Law: Offspring of Randomness at the Molecular Level / 182	
9.2	Fick's Second Law / 188	
9.3	Molecular Diffusivities / 194	
9.4	Turbulent Diffusion / 200	
10	THE GAS-LIQUID INTERFACE: AIR-WATER EXCHANGE	215
10.1	Introduction / 215	
10.2	Visualization of the Mechanisms Involved in Air-Water Exchange / 217	
10.3	Air-Water Exchange Model Formulations / 219	
10.4	Impact of Wind and Water Currents on v_w and v_a / 228	
10.5	Influence of Chemical Reactions on Air-Water Exchange Rates / 241	
10.6	Surface Films / 251	
11	SORPTION: SOLID-AQUEOUS SOLUTION EXCHANGE	255
11.1	Introduction / 255	
11.2	Quantifying the Relative Abundances of Dissolved and Sorbed Species: The Solid-Water Distribution Ratio K_d / 258	
11.3	The Complex Nature of K_d 's / 262	
11.4	Sorption of Neutral Organic Chemicals to Soils and Sediments / 265	
11.5	Sorption of Neutral Organic Chemicals to Polar Mineral Surfaces / 284	
11.6	Adsorption of Ionizable Organic Chemicals from Aqueous Solutions / 291	
11.7	Sorption Kinetics / 328	
12	CHEMICAL TRANSFORMATION REACTIONS	342
12.1	Introduction / 342	
12.2	Kinetic Aspects of Chemical Transformation Reactions / 344	
12.3	Nonreductive Chemical Reactions Involving Nucleophilic Species / 359	
12.4	Oxidation and Reduction Reactions / 399	
13	PHOTOCHEMICAL TRANSFORMATION REACTIONS	436
13.1	Introduction / 436	
13.2	Some Basic Principles of Photochemistry / 437	

13.3	Direct Photolysis of Organic Compounds in Natural Water / 451	
13.4	Indirect (Sensitized) Photolysis of Organic Compounds / 471	
13.5	Effects of Particles on Photolytic Transformations of Organic Compounds in Natural Water / 483	
14	BIOLOGICAL TRANSFORMATION REACTIONS	485
14.1	Introduction / 485	
14.2	Some Important Concepts about Microorganisms / 489	
14.3	Strategies of Microorganisms to Initiate Metabolism of Xenobiotic Compounds / 494	
14.4	Rates of Biotransformations / 520	
14.5	Closing Remarks / 546	
15	MODELING CONCEPTS	547
15.1	Introduction / 547	
15.2	Mass Balance—The Cornerstone of Box Models / 551	
15.3	Dynamic Box Models / 554	
15.4	The Solid–Water Interface: Modeling the Role of Particles / 578	
15.5	Space and Time: Continuous Models / 598	
	APPENDIX	617
	BIBLIOGRAPHY	626
	INDEX	657

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APPENDIX

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm)		Aqueous Solubility at 25°C (mol L ⁻¹)		Henry's Law Constant at 25°C (L atm mol ⁻¹)	Octanol-Water Partition Coefficient at 25°C [(mol L ⁻¹ octanol)/(mol L ⁻¹ water)]
					$-\log P^0$	$-\log P^0(L)$ (For Solids and Gases)	$-\log C_w^{sat}$	$-\log C_w^{sat}(L)$ (For Solids and Gases)		
<i>Saturated and Unsaturated Hydrocarbons</i>										
Methane	CH ₄	16.0	-182.5	-164.0		-2.44		0.38 ^a	2.82	1.09
Ethane	C ₂ H ₆	30.1	-183.3	-88.6		-1.60		1.09 ^a	2.69	1.81
Propane	C ₃ H ₈	44.1	-189.7	-42.1		-0.97		1.88 ^a	2.85	2.36
<i>n</i> -Butane	C ₄ H ₁₀	58.1	-138.4	-0.5		-0.39		2.98 ^a	2.98	2.89
<i>n</i> -Pentane	C ₅ H ₁₂	72.2	-129.7	36.1	0.16			3.25	3.09	3.62
<i>n</i> -Hexane	C ₆ H ₁₄	86.2	-95.0	69.0	0.69 *			3.83 ^a	3.14 ^{a*}	4.11
<i>n</i> -Heptane	C ₇ H ₁₆	100.2	-90.6	98.4	1.21			4.51	3.30	4.66
<i>n</i> -Octane	C ₈ H ₁₈	114.2	-56.8	125.7	1.73			5.20	3.47	5.18
<i>n</i> -Nonane	C ₉ H ₂₀	128.3	-51.0	150.8	2.24			5.94	3.70	
<i>n</i> -Decane	C ₁₀ H ₂₂	142.3	-29.7	174.1	2.76			6.57	3.81	
<i>n</i> -Dodecane	C ₁₂ H ₂₆	170.3	-9.6	216.3	3.80			7.52	3.72	
<i>n</i> -Hexadecane	C ₁₆ H ₃₄	226.4	18.2	287.0	5.73			7.80	2.07	
<i>n</i> -Octadecane	C ₁₈ H ₃₈	254.4	28.2	316.1	6.67			8.08	1.41	
Cyclohexane	C ₆ H ₁₂	84.2	6.6	80.7	0.90			3.15	2.25	3.44
1-Hexene	C ₆ H ₁₂	84.2	-139.8	63.4	0.60			3.15	2.45	3.39
1-Octene	C ₈ H ₁₆	112.2	-101.7	121.3	1.63			4.52	2.89	4.57
<i>Miscellaneous Aliphatic Compounds^c</i>										
1-Butanol	C ₄ H ₁₀ O	74.1	-89.5	117.2	2.02			0.07	-1.95	0.79
1-Hexanol	C ₆ H ₁₄ O	102.2	-46.7	158.0	2.85			0.88		2.03
1-Octanol	C ₈ H ₁₈ O	130.2	-16.7	194.4				2.35		2.84
1-Nonanol	C ₉ H ₂₀ O	144.2	-5.5	213.5	4.00			3.13		3.77
2-Ethyl-1,3-hexanediol	C ₈ H ₁₈ O ₂	146.2	-40.0	244.0				2.81		3.22
Cyclohexanol	C ₆ H ₁₂ O	100.2	25.1	161.1	2.70	2.70		0.42	-2.28	1.23
Acetone	C ₃ H ₆ O	58.1	-94.6	56.5	0.55			-1.13	-1.68	-0.24
									-1.44	

2-Octanone	$C_8H_{16}O$	128.2	-16.0	172.9	2.88	2.05	-0.83	2.76	
2-Decanone	$C_{10}H_{20}O$	156.2	3.5	211.0	3.45	3.30	-0.15	3.81	
<i>n</i> -Butylacetate	$C_6H_{12}O_2$	116.2	-77.9	126.5				1.78	
1-Bromohexane	$C_6H_{13}Br$	165.1	-84.7	155.3				4.65	
1-Bromoheptane	$C_7H_{15}Br$	179.1	-56.1	178.5				5.23	
1-Bromooctane	$C_8H_{17}Br$	193.1	-55.0	200.8		5.06		5.82	
Substituted Benzenes ^d									
Benzene	C_6H_6	78.1	5.5	80.1	0.90	1.64	0.74 (0.75 exp.)	2.13	
Toluene	C_7H_8	92.1	-95.0	110.6	1.42	2.25	0.83 (0.83 exp.)	2.69	
Ethylbenzene	C_8H_{10}	106.2	-95.0	136.2	1.90	2.80	0.90 (0.93 exp.)	3.15	
1,2-Dimethyl- benzene	C_8H_{10}	106.2	-25.2	144.4	2.05	2.76	0.71	3.12	
1,4-Dimethyl- benzene	C_8H_{10}	106.2	13.2	138.0	1.93	2.77	0.84	3.18	
<i>n</i> -Propylbenzene	C_9H_{12}	120.2	-101.6	159.2	2.35	3.34	0.99	3.63	
1,2,4-Tri- methylbenzene	C_9H_{12}	120.2	-43.8	169.4	2.57	3.33	0.76	3.65	
1,3,5-Tri- methylbenzene	C_9H_{12}	120.2	-44.7	164.7	2.48	3.40	0.92	3.42	
<i>n</i> -Butylbenzene	$C_{10}H_{14}$	134.2	-88.0	183.0	2.86	3.97	1.13	4.28	
<i>n</i> -Pentylbenzene	$C_{11}H_{16}$	148.3	-75.0	205.4	3.36	4.59	1.23	4.90	
Chlorobenzene	C_6H_5Cl	112.6	-45.6	132.0	1.80	2.35	0.55 (0.54 exp.)	2.92	
1,2-Dichloro- benzene	$C_6H_4Cl_2$	147.0	-17.0	180.0	2.71	3.20, 3.01	0.49, 0.29 (0.28 exp.)	3.38	
1,4-Dichloro- benzene	$C_6H_4Cl_2$	147.0	53.1	174.0	3.04	3.39	0.35	3.38	
1,2,4-Trichloro- benzene	$C_6H_3Cl_3$	181.5	16.9	213.5	3.21	3.65	0.44	4.00	
1,3,5-Trichloro- benzene	$C_6H_3Cl_3$	181.5	63.0	208.0	3.49	4.53	1.04	4.02	

Appendix (Continued)

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm)		Aqueous Solubility at 25°C (mol L ⁻¹)		Henry's Law Constant at 25°C (L atm mol ⁻¹)	Octanol-Water Partition Coefficient at 25°C [(mol L ⁻¹ octanol)/(mol L ⁻¹ water) ⁻¹]
					$-\log P^0$	$-\log P^0(L)$ (For Solids and Gases)	$-\log C_w^{sat}$	$-\log C_w^{sat}(L)$ (For Solids and Gases)		
1,2,3,4-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.9	47.5	254.0	4.28	4.06	4.42	4.20	0.14	4.55
1,2,3,5-Tetrachlorobenzene	C ₆ H ₂ Cl ₄	215.9	54.5	246.0	4.01	3.73	4.83	4.55	0.82	4.65
Pentachlorobenzene	C ₆ HCl ₅	250.3	86.0	277.0	4.66	4.05	5.56	4.95	0.90	5.03
Hexachlorobenzene	C ₆ Cl ₆	284.8	230.0	322.0	7.51	5.46	7.69	5.64	0.18	5.50
Bromobenzene	C ₆ H ₅ Br	157.0	-30.8	156.0	2.25	2.64	2.64		0.41	2.99
1,4-Dibromobenzene	C ₆ H ₄ Br ₂	235.9	87.3	219.0	3.67	3.05	4.07	3.45	0.40	3.75
4-Bromochlorobenzene	C ₆ H ₄ BrCl	191.5	68.0	196.0	3.46	3.03	3.63	3.20	0.17	3.53
Fluorobenzene	C ₆ H ₅ F	96.1	-41.2	85.1	1.00	1.00	1.79	0.79	0.79	2.27
Phenol	C ₆ H ₆ O	94.1	43.0	181.7	3.59	3.41	0.20	0.02	-3.39	1.45
3-Methyl phenol (<i>m</i> -cresol)	C ₇ H ₈ O	108.6	11.5	202.2			1.59			1.96
2,4-Dimethyl phenol	C ₈ H ₁₀ O	122.2	27.5	210.0			1.19	1.17		2.35
2-Chlorophenol	C ₆ H ₅ ClO	128.6	9.0	174.9			1.05			2.16
Aniline	C ₆ H ₇ N	93.1	-6.3	184.0	2.89		0.41		-2.48	0.90
<i>N</i> -Methylaniline	C ₇ H ₉ N	107.2	-57.0	196.3			1.28			1.66

Appendix (Continued)

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm)		Aqueous Solubility at 25°C (mol L ⁻¹)		Henry's Law Constant at 25°C (L-atm mol ⁻¹)	Octanol-Water Partition Coefficient at 25°C [(mol L ⁻¹ octanol)/(mol L ⁻¹ water)]
					$-\log P^0$	$-\log P^0(L)$ (For Solids and Gases)	$-\log C_w^{sat}$	$-\log C_w^{sat}(L)$ (For Solids and Gases)		
<i>Halogenated C₁-C₄ Compounds^a</i>										
Chloromethane	CH ₃ Cl	50.5	-97.7	-24.2	-0.76	0.98 ^a	0.22	0.98	0.91	
Dichloromethane	CH ₂ Cl ₂	84.9	-95.1	39.7	0.23	0.64		0.41 (0.43 exp.)	1.15	
Trichloromethane	CHCl ₃	119.4	-63.5	61.7	0.59	1.19		0.60 (0.59 exp.)	1.93	
Tetrachloromethane	CCl ₄	153.8	-22.9	76.5	0.82	2.20		1.38 (1.33 exp.)	2.73	
1,1-Dichloroethane	C ₂ H ₄ Cl ₂	99.0	-97.0	57.5	0.52	1.30		0.78	1.79	
1,2-Dichloroethane	C ₂ H ₄ Cl ₂	99.0	-35.4	83.5	1.04	1.07		0.03 (0.00 exp.)	1.47	
1,1,1-Trichloroethane	C ₂ H ₃ Cl ₃	133.4	-30.4	74.1	0.78	2.07		1.29	2.48	
1,1,2,2-Tetrachloroethane	C ₂ H ₂ Cl ₄	167.9	-36.0	146.2	2.06	1.74		-0.32	2.39	
Chloroethene (vinyl chloride)	C ₂ H ₃ Cl	62.5	-153.8	-13.4	-0.59	1.35 ^c	0.76	1.35	0.60	
Trichloroethene	C ₂ HCl ₃	131.4	-73.0	87.0	1.01	2.04		1.03	2.42	
Tetrachloroethene	C ₂ Cl ₄	165.8	-19.0	121.0	1.60	3.04		1.44	2.88	

Hexachloro-butadiene	C ₄ Cl ₆	260.8	-210	215.0	3.46 (calc)	4.90	1.44	4.90
Bromomethane	CH ₃ Br	94.9	-93.6	3.6		0.79 ^a	0.79	1.19
Tribromomethane	CHBr ₃	252.8	8.3	149.5	2.13	1.91	-0.22	
1,2-Dibromoethane	C ₂ H ₄ Br ₂	187.9	-34.2	167.3	2.57	2.04	-0.53	
1,2-Dibromo-3-chloropropane	C ₃ H ₅ Br ₂ Cl	236.4		178.0	2.90	2.44	-0.46	
Trichlorofluoromethane	CCl ₃ F	137.4	-111.0	23.8		2.10 ^a	2.10	2.16
Dichlorodifluoromethane	CCl ₂ F ₂	120.9	-158.0	-29.8		2.60 ^a	2.60	2.53

Polychlorinated Biphenyls (PCBs)^b

Biphenyl	C ₁₂ H ₁₀	154.2	71.0	255.9	5.00	3.88		4.09
2-CBP	C ₁₂ H ₉ Cl	188.6	32.1		4.66	4.57	-0.09	4.53
4-CBP	C ₁₂ H ₉ Cl	188.6	77.7		5.76	5.13	-0.63	4.40
2,5-CBP	C ₁₂ H ₈ Cl ₂	223.1	23.0		5.53	5.06	-0.47	5.22
4,4'-CBP	C ₁₂ H ₈ Cl ₂	223.1	149.0		7.32	6.53	-0.79	5.33
2,4,5-CBP	C ₁₂ H ₇ Cl ₃	257.5	76.3		6.95	6.26	-0.69	5.74
2',3,4-CBP	C ₁₂ H ₇ Cl ₃	257.5	60.0		6.88	6.52	-0.36	5.78
2,2',5,5'-CBP	C ₁₂ H ₆ Cl ₄	292.0	87.0		7.60	7.06	-0.54	6.18
2,3',4,4'-CBP	C ₁₂ H ₆ Cl ₄	292.0	128.0		8.21	7.70	-0.51	6.31
2,2',4,5,5'-CBP	C ₁₂ H ₅ Cl ₅	326.4	77.0		8.02	7.40	-0.62	6.36
2,2',4,4',5,5'-CBP	C ₁₂ H ₄ Cl ₆	360.9	103.0		8.97	7.82	-1.15	7.15
2,2',3,3',4,4'-CBP	C ₁₂ H ₄ Cl ₆	360.9	151.9		9.65	8.72	-0.93	6.97
2,2',3,3',4,4',6-CBP	C ₁₂ H ₃ Cl ₇	395.3	122.3		9.40	8.26	-1.14	6.68
2,2',3,3',5,5',6,6'-CBP	C ₁₂ H ₂ Cl ₈	429.8	161.0		9.54	9.29	-1.25	7.12
Decachloro-BP	C ₁₂ Cl ₁₀	498.7	305.8		12.28	10.55	-1.73	8.23

Appendix (Continued)

Compound Name	Molecular Formula	Mol. Wt.	T_m (°C)	T_b (°C)	Vapor Pressure at 25°C (atm)		Aqueous Solubility at 25°C (mol L ⁻¹)		Henry's Law Constant at 25°C (L atm mol ⁻¹)	Octanol-Water Partition Coefficient at 25°C [(mol L ⁻¹ octanol)/(mol L ⁻¹ water)]
					$-\log P^0$ (For Solids and Gases)	$-\log C_w^{sat}$ (For Solids and Gases)	$-\log C_w^{sat}$ (For Solids and Gases)	$-\log C_w^{sat}$ (For Solids and Gases)		
<i>Sulfur-Containing Compounds¹</i>										
Dimethyl sulfide	C ₂ H ₆ S	62.13	-98.0	37.3	0.20					
Diethyl sulfide	C ₄ H ₁₀ S	90.19	-103.8	92.1	1.12					1.95
Di- <i>n</i> -propyl sulfide	C ₆ H ₁₄ S	118.24	-102.5	142.4	2.10					
Diisopropyl sulfide	C ₆ H ₁₄ S	118.24	-78.1	120.0	1.72					
Dimethyl sulfide	C ₂ H ₆ S ₂	94.20	-84.7	109.7	1.42					1.77
Diethyl sulfide	C ₄ H ₁₀ S ₂	122.25	-101.5	154.0	2.20					
Thiophene	C ₄ H ₄ S	84.14	-38.2	84.2	0.98					1.81
2-Methyl thiophene	C ₅ H ₆ S	98.17	-63.4	112.6	1.46					
Methanethiol	CH ₄ S	48.11	-123.0	6.2						
Ethanethiol	C ₂ H ₆ S	62.13	-144.4	35.0	0.16	-0.300		0.091		
<i>n</i> -Propanethiol	C ₃ H ₈ S	76.17	-113.3	67.7	0.69					

Miscellaneous Pesticides and Other Compounds¹

2,3,7,8-Tetra-chlorodibenzo- <i>p</i> -dioxin	C ₁₂ H ₄ O ₂ Cl ₄	322.0	305	421	11.6	8.8	10.3	7.5	-1.3	6.64
Lindane (γ-hexa-chlorocyclohexane)	C ₆ H ₆ Cl ₆	290.8	112.9		7.08	6.20	4.59	3.71	-2.49	3.78
Dieldrin	C ₁₂ H ₈ Cl ₆ O	380.9	175.0		8.18	6.68	6.23	4.98	-1.95	5.48
<i>p,p'</i> -DDT	C ₁₄ H ₉ Cl ₅	354.5	109.0		9.87	9.03	7.85	7.01	-2.02	6.36
Parathion	C ₁₀ H ₁₄ NO ₃ PS	291.3	6.1		7.65		4.23		-3.42	3.81

Malathion	$C_{10}H_{19}O_6PS_2$	330.4	2.9		3.36		2.89
Phosmit	$C_{11}H_{12}NO_4PS_2$	317.3	72.0		4.10	3.63	2.83
Dialifos	$C_{14}H_{17}ClNO_4PS_2$	393.9	68.0	9.22 (20°C) 10.08 (30°C)	6.34	5.91	4.69
Carbaryl	$C_{12}H_{11}NO_2$	201.2	142.0		3.70	2.53	2.36
Carbofuran	$C_{12}H_{15}NO_3$	221.3	151.0		2.73	1.47	1.60
Fluometuron	$C_{10}H_{11}F_3NO_2$	232.2	164.0		3.51	1.39	1.34
Atrazine	$C_8H_{14}ClN_5$	215.7	174.0		3.81	2.33	2.56
RDX (1,3,5-triaza-1,3,5-trinitrocylohexane)	$C_3H_6N_6O_6$	222.1	205.0		4.57	2.77	0.87
Tributylphosphate	$C_{12}H_{27}PO_4$	266.3	<25		5.98		4.00
Tri- <i>o</i> -cresylphosphate	$C_{21}H_{21}PO_4$	368.4	77.0		6.01	5.49	5.11

^a At 1 atm.

^b Hansch and Leo (1979); Mackay and Shiu (1981); Stein (1981); Tewari et al. (1982).

^c Hansch and Leo (1979); CRC 1985-1986; Tewari et al. (1982).

^d Hansch and Leo (1979); Yalkowsky and Valvani (1979); Yalkowsky et al. (1979); Banerjee et al. (1980); CRC 1985-1986; Mackay and Shiu (1981); Chiu et al. (1982); Horvath (1982); Tewari et al. (1982); Miller et al. (1984).

^e Wauchope and Getzen (1972); Mackay et al. (1980a); May et al. (1983); Sonnefeld et al. (1983); Whitehouse (1984).

^f Wolfe et al. (1980); CRC 1985-1986; Leyder and Boulanger (1983).

^g Hansch and Leo (1979); Banerjee et al. (1980); Mackay and Shiu (1981); Horvath (1982).

^h Mackay et al. (1980b); Westcott et al. (1981); Bidleman (1984); Burkhard et al. (1984); Miller et al. (1984); Rapaport and Eisenreich (1984); Woodburn et al. (1984); Burkhard et al. (1985).

ⁱ Hansch and Leo (1979); CRC 1985-1986; Przyjazny et al. (1983).

^j Banerjee et al. (1980); Mackay and Shiu (1981); Lyman (1982a,b); Monsanto Company (1985); Marple et al. (1986a,b); Eitzer and Hites (1988).