

# **AQUEOUS SOLUBILITY**

## **METHODS OF ESTIMATION FOR ORGANIC COMPOUNDS**

**SAMUEL H. YALKOWSKY  
SUJIT BANERJEE**



6876

Marcel Dekker, Inc.

New York • Basel • Hong Kong

# ***Contents***

<b><i>Preface</i></b>	<b>iii</b>
<b><i>1. Introduction: Significance of Solubility</i></b>	
1.1 Solubility and Equilibrium Properties	1
1.2 Solubility and Kinetic Parameters	2
1.3 Solubility and Quantitative Structure-Activity Relationships	8
<b><i>2. Factors Influencing Solubility</i></b>	
2.1 Free Energy of Mixing	11
2.2 Enthalpy of Mixing	12
2.3 Entropy of Mixing	13
2.4 Liquid Solutes	18
2.5 Solid Solutes	19
2.6 The Solute Phase	31
2.7 Temperature Effects	38
2.8 Pressure Effects	40
<b><i>3. Estimation of Aqueous Solubility</i></b>	
3.1 Classification of Methods	41
3.2 Group Activity Coefficients	42
3.3 Partition Coefficients	51
3.4 Chromatographic Parameters	68
3.5 Boiling Point	74

3.6	Molecular Volume	75
3.7	Molecular Surface Area	87
3.8	Molecular Connectivity	97
3.9	Parachor	100
3.10	Solubility Parameters	104
3.11	UNIFAC	107
3.12	Linear Solvation Energy	117
3.13	Multivariate Statistical Methods	124
<b>4.</b>	<b><i>Comparison of Methods</i></b>	
4.1	Classification of Parameters	128
4.2	Regression and Prediction	131
4.3	Intercorrelation Among Parameters (Training Set)	132
4.4	Intercorrelation Among Parameters (Test Set)	141
4.5	Recommended Methods for Estimating the Aqueous Activity Coefficient	144
<b>5.</b>	<b><i>Measurement, Evaluation and Sources of Solubility</i></b>	
5.1	Measurement of Solubility	149
5.2	Sources of Solubility Data	154
<b><i>Appendices</i></b>		
A.	Glossary of Abbreviations	156
B.	Computer Program for UNIFAC Calculations	158
C.	Solubilities of Some Superfund "Extremely Hazardous Substances"	191
<b><i>References</i></b>		232
<b><i>Index</i></b>		255