



Chemical Property Estimation: Theory and Application

Edward Baum

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Our world is widely contaminated with damaging chemicals, and companies create thousands of new, potentially dangerous chemicals each year. Due to the difficulty and expense of obtaining accurate measurements and the unreliability of reported values, we know surprisingly little about the properties of these contaminants. Determining the properties of chemicals is critical to judging their impact on environmental quality and in making decisions about emission rates, clean-up, and other important public health issues.

Chemical Property Estimation describes modern methods of estimating chemical properties, methods which cost much less than traditional laboratory techniques and are sufficiently accurate for most environmental applications. Estimation methods are used to screen chemicals for testing, design monitoring and analysis methods, design clean-up procedures, and verify experimental measurements. The book discusses key methods for estimating chemical properties and considers their relative strengths and weaknesses. Several chapters are devoted to the partitioning of chemicals between air, water, soil, and biota; and properties such as solubility, vapor pressure, and chemical transport.

Each chapter begins with a review of relevant theory and background information explaining the applications and limitations of each method. Sample calculations and practical advice on how and when to use each method are included as well. Each method is evaluated for accuracy and reliability. Computer software, databases, and internet resources are evaluated, as well as other supplementary material, such as fundamental constants, units of measure, and more.

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