The octanol-water partition coefficient is a laboratory-measured property of a substance. It provides a thermodynamic measure of the tendency of the substance to prefer a non-aqueous or oily milieu rather than water (i.e. its hydrophilic/lipophilic balance). Partition coefficients are used extensively in medicinal chemistry, drug design, ecotoxicology and environmental chemistry. The partition coefficient is recognized by governmental and international agencies (U.S. Environmental Protection Agency, OECD) as a physical property of organic pollutants equal in importance to vapour pressure, water solubility and toxicity. Octanol-Water Partition Coefficients is a comprehensive and up-to-date survey of the thermodynamics of partitioning and of the octanol-water pair. In addition, all current methods of measurement are reviewed, strengths and weaknesses are noted and recommendations for particular applications are given. Current methods of calculation of partition coefficients are similarly surveyed and described. Five of the most popular computerized methods are tested for predictive accuracy for drugs, pollutants, aminoacids, etc. The book will be of interest not only to solution chemists, but to any chemists who use partition coefficients. It provides a thorough understanding of the fundamentals and offers clear guidance on the choice of methods of measurement and calculation. Contents: Introduction, Thermodynamics and Extrathermodynamics of Partitioning, Experimental Methods of Measurement, Discussion of Measurement Methods, Methods of Calculating Partitioning Coefficients, Discussion of LogKow Predictive Methods The Wiley Series in Solution Chemistry fills the increasing need to present authoritative, comprehensive and fully up-to-date accounts of the many aspects of solution chemistry. Internationally recognized experts from research or teaching institutions in various countries are invited to contribute to the series.
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