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Book Description. A complete restructuring and updating of the classic 1982 Handbook of Chemical Property Estimation Methods (commonly known as "Lyman's Handbook"), the Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences reviews and recommends practical methods for estimating environmentally important properties of organic chemicals.

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A complete restructuring and updating of the classic 1982 Handbook of Chemical Property Estimation Methods (commonly known as "Lyman's Handbook"), the Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences reviews and recommends practical methods for estimating environmentally important properties of organic chemicals. One of the most eagerly anticipated revisions in scientific publishing, the new Handbook includes both a foreword and a chapter by Dr. Lyman. Written for convenient and frequent use, each chapter integrates recent developments while retaining the elements that made the first version a classic. As a reference tool, the New Edition is indispensable. It comprehensively reviews recent developments in chemical property estimation methods and focuses on the properties most critical to environmental fate assessment.

Octanol/water partition coefficient. Solubility in water. Solubility in various solvents. Adsorption coefficient for soils and sediments. Bioconcentration factor in aquatic organisms. Acid association constant. Rate of hydrolysis. Rate of aqueous photolysis. Rate of biodegradation. Atmospheric residence time. Activity coefficient. Boiling point. Heat of vaporization. Vapor pressure. Volatilization from water. Volatilization from soil. Diffusion coefficients in air and water. Flash points of pure substances. Densities of vapors, liquids and solids. Surface tension. Interfacial tension with water. Liquid viscosity. Heat capacity. Thermal conductivity. Dipole moment. Index of refraction. Simple linear regression. Evaluating propagated and total error in chemical property estimates.

After seven years, a revision of the "Handbook of Chemical Property Estimation Methods" (commonly known as "Lyman's Handbook") is finally complete. The 1999 publication of that revision, entitled Handbook of Property Estimation Methods for Environmental and Health Sciences, is one of the most eagerly anticipated developments in scientific publishing. This is a completely new book, but it includes both a foreword and a chapter by Dr. Lyman.

A complete restructuring and updating of the classic 1982 Handbook of Chemical Property Estimation Methods (commonly known as "Lyman's Handbook"), the Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences reviews and recommends practical methods for estimating environmentally important properties of organic chemicals. One of the most eagerly anticipated revisions in scientific publishing, the new Handbook includes both a foreword and a chapter by Dr. Lyman. Written for convenient and frequent use, each chapter integrates recent developments while retaining the elements that made the first version a classic. As a reference tool, the New Edition is indispensable. It comprehensively reviews recent developments in chemical property estimation methods and focuses on the properties most critical to environmental fate assessment.

A comprehensive compendium of published property estimation techniques for organic compounds. For scientists and engineers seeking to estimate properties of compounds, this time-saving Handbook brings together in one compact volume a vast array of property estimation methods from more than 2,700 published sources for calculating these and many other properties of organic compounds: \* Density and molar volume \* Boiling point \* Refractive index and molar refraction \* Melting point \* Surface tension and parachor \* Water solubility \* Viscosity \* \* Air/water partition coefficient \* Vapor pressure \* Octanol/water partition coefficient \* Enthalpy of vaporization \* Soil/water partition coefficient. The property estimation techniques detailed in the Handbook have been chosen for their broad applicability and practical value. The discussion of each estimating technique includes a clear exposition of the technique, including classes of compounds for which it is applicable and critical consideration of its strengths and weaknesses, as well as many worked-out examples demonstrating the technique. The Handbook can be used on its own or in tandem with the Toolkit for Estimating Physicochemical Properties of Organic Compounds, an easy-to-use, Windows(r)-based program that puts rapid estimation routines and flexible search capabilities at the user's fingertips. The Toolkit CD features routines for estimating key properties of organic compounds and a database of property and other data for more than 24,000 organic compounds. Also available: Toolkit for Estimating Physicochemical Properties of Organic Compounds ISBN 0-471-17263-4 (book/CD-ROM set)

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.

Quick access to data and fast property estimation techniques for organic compounds. An invaluable time-saver for busy scientists and researchers, the Toolkit uses algorithms derived from more than 2,700 published sources to calculate these key properties of organic compounds quickly and easily: \* Density and molar volume \* Boiling point \* Refractive index and molar refraction \* Melting point \* Surface tension and parachor \* Water solubility \* Viscosity \* Air/water partition coefficient \* Vapor pressure \* Octanol/water partition coefficient \* Enthalpy of vaporization \* Soil/water partition coefficient. These properties can be estimated using published methods and, in some cases, temperature-dependent functions. Complete bibliographic citations are included for each property estimation technique, and properties are simultaneously retrieved for approximately 24,000 organic compounds, most of them derived from the Registry of Physicochemical Data. The Toolkit is flexible and easy-to-use, allowing the user to perform structure and database searches. It contains EndNote 3 Demo Version for searching and viewing an extensive bibliography comprising more than 2,700 references. Structures can be created in CS ChemDrawNet or imported via clipboard function from other chemical drafting programs using MDL MOLfile format, or imported from disk as MDL MOLfiles. Minimum system requirements: IBM-compatible PC 486 \* Win95(r) or higher \* CD-ROM drive and 8MB RAM \* 18MB free hard disk space for minimum installation. CS ChemDrawNet is a registered trademark of CambridgeSoft Corporation. EndNote 3 is a registered trademark of Niles Software, Inc. Registry of Physicochemical Data is a trademark of Synexchem Consulting Services International, LLC. Also available: \* Handbook for Estimating Physicochemical Properties of Organic Compounds Toolkit for Estimating Physicochemical Properties of Organic Compounds

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