

CHEMICAL PROPERTY ESTIMATION

Theory and Application



Edward J. Baum

Chemical Property Estimation

Clark D. Linde



Chemical Property Estimation:

Chemical Property Estimation Edward Baum, 2018-05-11 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

Handbook of Property Estimation Methods for Chemicals Donald Mackay, Robert S. Boethling, 2000-03-29 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 [Handbook of Chemical Property Estimation Methods](#) Warren J. Lyman, 1990

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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 **User's Guide CHEMEST** Warren J. Lyman, Michael Callahan, Richard G. Potts, Gary C. Magil, United States. Environmental Protection Agency. Office of Pesticides and Toxic Substances, US Army Medical Bioengineering Research and Development Laboratory. Environmental Protection Research Division, Arthur D. Little, Inc, 1984 **Handbook of Chemical property estimation methods**, 1981

Handbook for Estimating Physicochemical Properties of Organic Compounds Martin Reinhard, Axel Drefahl, 1999 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 many properties of organic compounds 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 **Computer Aided Property Estimation for Process and Product Design** Georgios M. Kontogeorgis, Rafiqul Gani, 2004-06-30 Properties of chemical compounds and their mixtures are needed in almost every aspect of process and product design When the use of experimental data is not possible one of the most widely used options in the use of property estimation models Computer Aided Property Estimation for Process and Product Design provides a presentation of the most suitable property estimation models available today as well as guidelines on how to select an appropriate model Problems that users are faced with such as which models to use and what their accuracy is are addressed using a systematic approach to property estimation The volume includes contributions from leading experts from academia and industry A wide spectrum of properties and phase equilibria types is covered making it indispensable for research development and educational purposes This book presents the latest developments in computational modelling for thermodynamic property estimation It combines theory with practice and includes illustrative examples of software applications The questions users of property models are faced with are addressed comprehensively

AIChE Physical Property Estimation System American Institute of Chemical Engineers, 1945 *Application of Structure-activity Relationships to the Estimation of Properties Important in Exposure Assessment*, 1993 **Chemical Engineering** Louis Theodore, 2013-10-14 A practical concise guide to chemical engineering principles and applications Chemical Engineering The Essential Reference is the condensed but authoritative chemical engineering reference boiled down to principles and hands on skills needed to solve real world problems Emphasizing a pragmatic approach the book delivers critical content in a convenient format and presents on the job topics of importance to the chemical engineer of

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