

A New Group Contribution Method For The Estimation Of

Charles Frederick Askonas

Development of a Second-order Group Contribution Method for the Estimation of Pure Component Vapor Pressure
Charles Frederick Askonas, 1986

Vapor-Liquid Equilibria Using Unifac Aage Fredenslund, 2012-12-02 *Vapor-Liquid Equilibria Using UNIFAC: A Group-Contribution Method* focuses on the UNIFAC group-contribution method used in predicting quantitative information on the phase equilibria during separation by estimating activity coefficients. Drawing on tested vapor-liquid equilibrium data on which UNIFAC is based, it demonstrates through examples how the method may be used in practical engineering design calculations. Divided into nine chapters, this volume begins with a discussion of vapor and liquid phase nonidealities and how they are calculated in terms of fugacity and activity coefficients, respectively. It then introduces the reader to the UNIFAC method and how it works, the procedure used in establishing the parameters needed for the model, prediction of binary and multicomponent vapor-liquid equilibria for a large number of systems, the potential of UNIFAC for predicting liquid-liquid equilibria, and how UNIFAC can be used to solve practical distillation design problems. This book will benefit process design engineers who want to reliably predict phase equilibria for designing distillation columns and other separation processes.

Properties of Polymers D.W. van Krevelen, 2012-12-02 *Properties of Polymers: Their Correlation with Chemical Structure; Their Numerical Estimation and Prediction from Additive Group Contributions* summarizes the latest developments regarding polymers, their properties in relation to chemical structure, and methods for estimating and predicting numerical properties from chemical structure. In particular, it examines polymer electrical properties, magnetic properties, and mechanical properties, as well as their crystallization and environmental behavior and failure. The rheological properties of polymer melts and polymer solutions are also considered. Organized into seven parts encompassing 27 chapters, this book begins with an overview of polymer science and engineering, including the typology of polymers and their properties. It then turns to a discussion of thermophysical properties, from transition temperatures to volumetric and calorimetric properties, along with the cohesive aspects and conformation statistics. It also introduces the reader to the behavior of polymers in electromagnetic and mechanical fields of force. The book covers the quantities that influence the

transport of heat, momentum, and matter, particularly heat conductivity, viscosity, and diffusivity; properties that control the chemical stability and breakdown of polymers; and polymer properties as an integral concept, with emphasis on processing and product properties. Readers will find tables that give valuable (numerical) data on polymers and include a survey of the group contributions (increments) of almost every additive function considered. This book is a valuable resource for anyone working on practical problems in the field of polymers, including organic chemists, chemical engineers, polymer processors, polymer technologists, and both graduate and PhD students.

Computer Aided Molecular Design Luke Achenie, Venkat Venkatasubramanian, Rafiqul Gani, 2002-11-20 CAMD or Computer Aided Molecular Design refers to the design of molecules with desirable properties. That is, through CAMD, one determines molecules that match a specified set of (target) properties. CAMD as a technique has a very large potential as in principle, all kinds of chemical, bio-chemical and material products can be designed through this technique. This book mainly deals with macroscopic properties and therefore does not cover molecular design of large, complex chemicals such as drugs. While books have been written on computer aided molecular design relating to drugs and large complex chemicals, a book on systematic formulation of CAMD problems and solutions, with emphasis on theory and practice, which helps one to learn, understand and apply the technique is currently unavailable. This title brings together the theoretical aspects related to Computer Aided Molecular Design, the different techniques that have been developed and the different applications that have been reported. Contributing authors are among the leading researchers and users of CAMD. First book available giving a systematic formulation of CAMD problems and solutions

A New Class of Group Contribution Based Property Estimation Methods for Process Modelling and Design J. Abildskov, R. Gani, American Institute of Chemical Engineers, 1996

Drug-like Properties: Concepts, Structure Design and Methods Li Di, Edward H Kerns, 2010-07-26 Of the thousands of novel compounds that a drug discovery project team invents and that bind to the therapeutic target, typically only a fraction of these have sufficient ADME/Tox properties to become a drug product. Understanding ADME/Tox is critical for all drug researchers, owing to its increasing importance in advancing high quality candidates to clinical studies and the processes of drug discovery. If the properties are weak, the candidate will have a high risk of failure or be less desirable as a drug product. This book is a tool and resource for scientists engaged in, or preparing for, the selection and optimization process. The authors describe how properties affect in vivo pharmacological activity and impact in vitro assays. Individual drug-like properties are discussed from a practical point of view, such as solubility, permeability and metabolic stability, with regard to fundamental understanding, applications of property data in drug discovery and examples of structural modifications that have achieved improved property performance. The authors also review various methods for the screening (high throughput), diagnosis (medium throughput) and in-depth (low throughput) analysis of drug properties. - Serves as an essential working

handbook aimed at scientists and students in medicinal chemistry - Provides practical, step-by-step guidance on property fundamentals, effects, structure-property relationships, and structure modification strategies - Discusses improvements in pharmacokinetics from a practical chemist's standpoint

Handbook of Chemical Engineering Calculations Nicholas P. Chopey, 1994 A compilation of the calculation procedures needed every day on the job by chemical engineers. Tables of Contents: Physical and Chemical Properties; Stoichiometry; Phase Equilibrium; Chemical-Reaction Equilibrium; Reaction Kinetics and Reactor Design; Flow of Fluids and Solids; Heat Transfer; Distillation; Extraction and Leaching; Crystallization; Filtration; Liquid Agitation; Size Reduction; Drying; Evaporation; Environmental Engineering in the Plant. Illustrations. Index.

Thermodynamics of Biochemical Reactions Robert A. Alberty, 2005-01-28 Ein Lehr- und Handbuch der Thermodynamik biochemischer Reaktionen mit modernen Beispielen und umfangreichen Hinweisen auf die Originalliteratur. - Schwerpunkt liegt auf Stoffwechsel und enzymkatalysierten Reaktionen - Grundlagen der Thermodynamik (z. B. chemisches Gleichgewicht) werden anschaulich abgehandelt - zu den speziellen Themen gehören Reaktionen in Matrices, Komplexbildungsgleichgewichte und Ligandenbindung, Phasengleichgewichte, Redoxreaktionen, Kalorimetrie

CRC Handbook of Thermophysical and Thermochemical Data David R. Lide, Henry V. Kehiaian, 2020-09-23 The CRC Handbook of Thermophysical and Thermochemical Data is an interactive software and handbook package that provides an invaluable source of reliable data embracing a wide range of properties of chemical substances, mixtures, and reacting systems. Use the handbook and software together to quickly, and easily generate property values at any desired temperature, pressure, or mixture composition.

Hansen Solubility Parameters Charles M. Hansen, 2007-06-15 Hansen solubility parameters (HSPs) are used to predict molecular affinities, solubility, and solubility-related phenomena. Revised and updated throughout, Hansen Solubility Parameters: A User's Handbook, Second Edition features the three Hansen solubility parameters for over 1200 chemicals and correlations for over 400 materials including p

The SAGE Encyclopedia of Communication Research Methods Mike Allen, 2017-04-11 Communication research is evolving and changing in a world of online journals, open-access, and new ways of obtaining data and conducting experiments via the Internet. Although there are generic encyclopedias describing basic social science research methodologies in general, until now there has been no comprehensive A-to-Z reference work exploring methods specific to communication and media studies. Our entries, authored by key figures in the field, focus on special considerations when applied specifically to communication research, accompanied by engaging examples from the literature of communication, journalism, and media studies. Entries cover every step of the research process, from the creative development of research topics and questions to literature reviews, selection of best methods (whether quantitative, qualitative, or mixed) for

analyzing research results and publishing research findings, whether in traditional media or via new media outlets. In addition to expected entries covering the basics of theories and methods traditionally used in communication research, other entries discuss important trends influencing the future of that research, including contemporary practical issues students will face in communication professions, the influences of globalization on research, use of new recording technologies in fieldwork, and the challenges and opportunities related to studying online multi-media environments. Email, texting, cellphone video, and blogging are shown not only as topics of research but also as means of collecting and analyzing data. Still other entries delve into considerations of accountability, copyright, confidentiality, data ownership and security, privacy, and other aspects of conducting an ethical research program. Features: 652 signed entries are contained in an authoritative work spanning four volumes available in choice of electronic or print formats. Although organized A-to-Z, front matter includes a Reader's Guide grouping entries thematically to help students interested in a specific aspect of communication research to more easily locate directly related entries. Back matter includes a Chronology of the development of the field of communication research; a Resource Guide to classic books, journals, and associations; a Glossary introducing the terminology of the field; and a detailed Index. Entries conclude with References/Further Readings and Cross-References to related entries to guide students further in their research journeys. The Index, Reader's Guide themes, and Cross-References combine to provide robust search-and-browse in the e-version.

Discrete Choice Methods with Simulation Kenneth Train, 2009-07-06 This book describes the new generation of discrete choice methods, focusing on the many advances that are made possible by simulation. Researchers use these statistical methods to examine the choices that consumers, households, firms, and other agents make. Each of the major models is covered: logit, generalized extreme value, or GEV (including nested and cross-nested logits), probit, and mixed logit, plus a variety of specifications that build on these basics. Simulation-assisted estimation procedures are investigated and compared, including maximum stimulated likelihood, method of simulated moments, and method of simulated scores. Procedures for drawing from densities are described, including variance reduction techniques such as antithetics and Halton draws. Recent advances in Bayesian procedures are explored, including the use of the Metropolis-Hastings algorithm and its variant Gibbs sampling. The second edition adds chapters on endogeneity and expectation-maximization (EM) algorithms. No other book incorporates all these fields, which have arisen in the past 25 years. The procedures are applicable in many fields, including energy, transportation, environmental studies, health, labor, and marketing.

Maximum Likelihood Estimation for Sample Surveys Raymond L. Chambers, David G. Steel, Suojin Wang, Alan Welsh, 2012-05-02 Sample surveys provide data used by researchers in a large range of disciplines to analyze important relationships using well-established and widely used likelihood methods. The methods used to select samples often result in the sample differing in important ways from the target population and standard application of likelihood methods can lead to

biased and inefficient estimates. Maximum Likelihood Estimation for Sample Surveys presents an overview of likelihood methods for the analysis of sample survey data that account for the selection methods used, and includes all necessary background material on likelihood inference. It covers a range of data types, including multilevel data, and is illustrated by many worked examples using tractable and widely used models. It also discusses more advanced topics, such as combining data, non-response, and informative sampling. The book presents and develops a likelihood approach for fitting models to sample survey data. It explores and explains how the approach works in tractable though widely used models for which we can make considerable analytic progress. For less tractable models numerical methods are ultimately needed to compute the score and information functions and to compute the maximum likelihood estimates of the model parameters. For these models, the book shows what has to be done conceptually to develop analyses to the point that numerical methods can be applied. Designed for statisticians who are interested in the general theory of statistics, Maximum Likelihood Estimation for Sample Surveys is also aimed at statisticians focused on fitting models to sample survey data, as well as researchers who study relationships among variables and whose sources of data include surveys.

Ecological Inference Gary King, Martin A. Tanner, Ori Rosen, 2004-09-13 Drawing upon the recent explosion of research in the field, a diverse group of scholars surveys the latest strategies for solving ecological inference problems, the process of trying to infer individual behavior from aggregate data. The uncertainties and information lost in aggregation make ecological inference one of the most difficult areas of statistical inference, but these inferences are required in many academic fields, as well as by legislatures and the Courts in redistricting, marketing research by business, and policy analysis by governments. This wide-ranging collection of essays offers many fresh and important contributions to the study of ecological inference.

Age Estimation Joe Adserias-Garriga, 2019-04-11 Age Estimation: A Multidisciplinary Approach is the only reference in the field covering all techniques and methods involving age estimation from different perspectives in just one volume. The book provides comprehensive coverage of all aspects of age estimation: aging the living and the dead, human rights, and skeletal, dental, histological and biochemical techniques and methods available. Each chapter is written by internationally known expert contributors. Age Estimation: A Multidisciplinary Approach is a one of a kind resource for those involved in estimating the age of the living and the dead. - Presents a concentration of all techniques and methods involving age estimation in a single volume - Provides a multidisciplinary approach that lends itself to researchers, practitioners and students from a variety of different fields - Includes contributions by world renowned forensic specialists

Selected Values of Properties of Hydrocarbons Frederick Dominic Rossini, American Petroleum Institute. Research Project 44, 1947

Materials Science of Membranes for Gas and Vapor Separation Benny Freeman, Yuri Yampolskii, Ingo

Pinnau,2006-05-12 *Materials Science of Membranes for Gas and Vapor Separation* is a one-stop reference for the latest advances in membrane-based separation and technology. Put together by an international team of contributors and academia, the book focuses on the advances in both theoretical and experimental materials science and engineering, as well as progress in membrane technology. Special attention is given to comparing polymer and inorganic/organic separation and other emerging applications such as sensors. This book aims to give a balanced treatment of the subject area, allowing the reader an excellent overall perspective of new theoretical results that can be applied to advanced materials, as well as the separation of polymers. The contributions will provide a compact source of relevant and timely information and will be of interest to government, industrial and academic polymer chemists, chemical engineers and materials scientists, as well as an ideal introduction to students.

Viscosity of Liquids Dabir S. Viswanath,Tushar K. Ghosh, Dasika H.L. Prasad,Nidamarty V.K. Dutt,Kalipatnapu Y. Rani,2007-03-31 This book is unique in that it brings together published viscosity data, experimental methods, theoretical, correlation and predictive procedures in a single volume. The readers will get a better understanding of why various methods are used for measuring viscosity of different types of liquids and why an experimental method is dependent on fluid characteristics, such as Newtonian or non-Newtonian fluids.

Chemical Product Design: Towards a Perspective through Case Studies Ka M. Ng,Rafiqul Gani,Kim Dam-Johansen,2006-10-24 *Chemical Product Design: Towards a Perspective through Case Studies* provides a framework for chemical product design problems which are clearly defined together with different solution approaches. This book covers the latest methods and tools currently available in the field and discusses future challenges that the chemical industry is faced with. It focuses on important issues of chemical product design and provides a good overview on industrial chemical product design problems through case studies supplied by leading experts. The editors of *Chemical Product Design* teach chemical product design at graduate level courses and also serve as consultants for various chemical companies. They have also developed experimental techniques for chemical product design as well as computer-aided design methods and tools. - Highlights important issues of chemical product design through case studies - Case studies supplied by leading experts in chemical product design - Provides a complete framework for chemical product design

10th International Symposium on Process Systems Engineering Rita Maria de Brito Alves,Cláudio Augusto Oller do Nascimento,Evaristo Chalbaud Biscaia (Jr),2009 The 10th International Symposium on Process Systems Engineering, PSE'09, will be held in Salvador-Bahia, Brazil on August 16-20, 2009. The special focus of PSE 2009 is Sustainability, Energy and Engineering. PSE 2009 is the tenth in the triennial series of international symposia on process systems engineering initiated in 1982. The meeting is brings together the worldwide PSE community of researchers and practitioners who are involved in the creation and application of computing-based methodologies for planning, design, operation, control and maintenance of

chemical and petrochemical process industries. PSE'09 will look at how the PSE methods and tools can support sustainable resource systems and emerging technologies in the areas of green engineering: environmentally conscious design of industrial processes. PSE methods and tools support: - sustainable resource systems - emerging technologies in the areas of green engineering - environmentally conscious design of industrial processes

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