



Soil/Sediment Adsorption Constant Program PCKOC



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Soil Sediment Adsorption Constant Program

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Soil Sediment Adsorption Constant Program:

Soil/Sediment Adsorption Constant Program Philip H. Howard, William M. Meylan, 1992-06-26 Soil Sediment Adsorption Constant Program uses the SMILES notation structural input to calculate the soil or sediment adsorption coefficient K_{oc} from a correlation of the molecular connectivity indices and correction factors for certain chemical classes This method was developed by the U S Environmental Protection Agency's EPA Office of Toxic Substances and is now available for use on any IBM or IBM compatible computer with 240K RAM This powerful user friendly program provides reliable data that will benefit any environmental chemist or regulator chemical companies and analytical labs *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 for Estimating Physico-chemical Properties of Organic Compounds Axel Drefahl, Martin Reinhard, 1995
Environmental Health Perspectives ,2003-07 **Best Practicable Environmental Option Assessments for**

Integrated Pollution Control Great Britain. Environment Agency, 1997 **Boletín de la Sociedad Internacional de la Ciencia Del Suelo** International Society of Soil Science, 1993 Computer Generated Physical Properties Stan Bumble, 1999-06-01 *Computer Generated Physical Properties* offers the environmental scientist a basis to predict the properties of molecules and reengineer them to remove those properties that are harmful to the environment This technology is currently used in other fields and is now becoming popular in the environmental engineering field because of its pollution prevention and waste reduction capabilities This book interdisciplinary in scope treats the physical properties of matter as generated by computers It covers a wide variety of topics pointing towards synthesizing new molecules to substitute for

reactants intermediaries and products in industrial processes with better physical and environmental properties than the original The author achieves this with a spreadsheet program called SYNPROPS that operates on a PC computer with optimization features A radar type graph one for each property visually sorts the various groups in order of their contribution to the property creating the necessity for a computer to obtain answers for the structure of the optimum molecules for substitution or synthesis The author discusses applications to biologically active molecules without side effects including antineoplastic drugs Additionally he demonstrates model compounds and the applications of SYNPROPS optimization and substitution This book has everything you need to know about deriving properties and combinational chemistry from molecular structure

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