

Unveiling the Secrets of pKa Prediction: Computational Approaches for Environmental QSAR



Unlocking the Power of pKa Values for Environmental Understanding

pKa values, a measure of a molecule's acidity or basicity, hold immense significance in various environmental processes. From predicting the fate and transport of chemicals to understanding their interactions with biological systems, pKa values serve as fundamental descriptors in environmental research and modeling.

Computational Approaches for the Prediction of pKa Values QSAR in Environmental Science presents state-of-the-art computational methods for accurately predicting pKa values of organic compounds. This book offers a comprehensive guide to the theory, algorithms, and applications of quantitative structure-activity relationship (QSAR) models for pKa prediction.



Computational Approaches for the Prediction of pKa Values (QSAR in Environmental and Health Sciences Book 4) by George C. Shields

★★★★☆ 4.1 out of 5

Language : English

File size : 4995 KB

Screen Reader : Supported

Print length : 175 pages



Unveiling the Secrets of pKa Prediction with QSAR

QSAR models establish mathematical relationships between molecular structure and properties, enabling the prediction of pKa values based on molecular descriptors. This book provides a deep dive into:

- The basics of QSAR modeling, including linear regression, nonlinear regression, and machine learning techniques
- Various molecular descriptors used for pKa prediction, including constitutional, topological, geometrical, and electronic properties
- Advanced QSAR modeling approaches, such as ensemble modeling, artificial neural networks, and genetic algorithms

Exploration of Real-World Applications

The book showcases the practical applications of pKa prediction in environmental science, including:

- Predicting the fate and transport of pollutants in soil and water
- Assessing the toxicity and bioavailability of chemicals
- Designing greener chemicals and materials

A Valuable Resource for Environmental Scientists and Researchers

Computational Approaches for the Prediction of pKa Values QSAR in Environmental Science is an invaluable resource for environmental scientists, QSAR modelers, and researchers seeking to understand and predict the behavior of chemicals in the environment. It provides a comprehensive overview of the current state of the field and sets the stage for future advancements in pKa prediction.

Free Download Your Copy Today!

Get your copy of this groundbreaking book and unlock the power of pKa prediction for environmental understanding.

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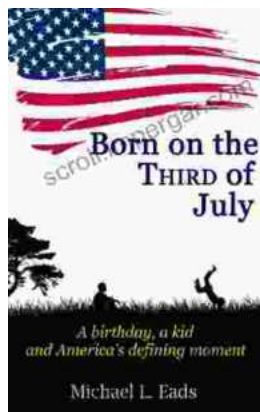
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