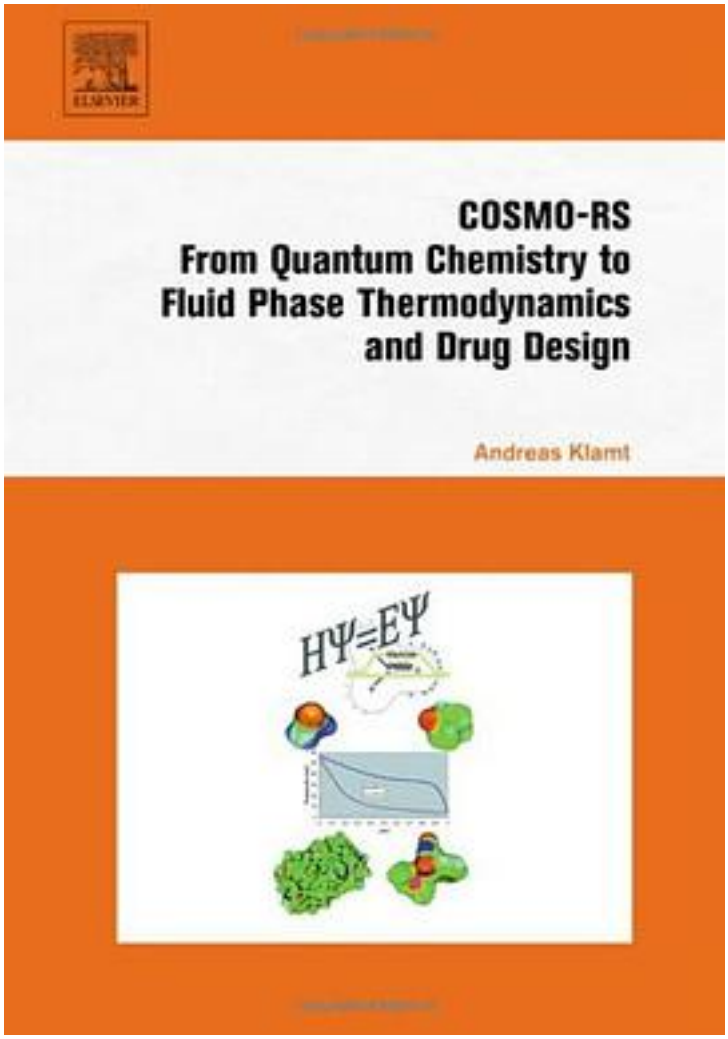
COSMO-RS



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The COSMO-RS technique is a novel method for predicting the thermodynamic

properties of pure and mixed fluids which are important in many areas, ranging from chemical engineering to drug design. "COSMO-RS, From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design" is about this novel technology, which has recently proven to be the most reliable and efficient tool for the prediction of vapour-liquid equilibria. In contrast to group contribution methods, which depend on an extremely large number of experimental data, COSMO-RS calculates the thermodynamic data from molecular surface polarity distributions, resulting from quantum chemical calculations of the individual compounds in the mixture. In this book, the author cleverly combines a vivid overview of the partly demanding theoretical steps with a deeper analysis of their scientific background and justification. Aimed at theoretical chemists, computational chemists, physical chemists, chemical engineers, thermodynamicists as well as students,academic and industrial experts, "COSMO-RS, From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design" provides a novel viewpoint to anyone looking to gain more insight into the theory and potential of the unique method, COSMO-RS. Readers can study many of the examples given using the accompanying demonstration CD of the COSMOtherm program, which also contains the DFT/COSMO files of common chemicals and the compounds described in the book. This is the only book currently available on COSMO-RS technique. It provides a novel viewpoint for the scientific understanding and for the practical quantitative treatment of fluid phase thermodynamics. It includes illustrative examples and an accompanying CD of the COSMOtherm program.

作者介绍:

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