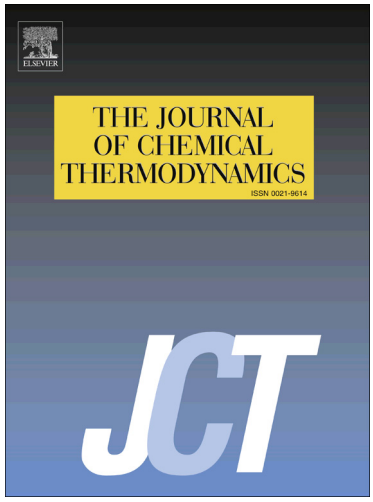

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Redefining Solubility Parameters: Bulk and Surface Properties from Unified Molecular Descriptors

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ABSTRACT

The central objective of this work is to revisit the development of the widely used solubility parameters and linear solvation energy relationships (LSER) and seek interconnections and possibilities for secure exchange of information. Partial solvation parameters (PSP) are used as the reference concept through which the unification is attempted and extended to surface tension components. Simple expressions are reported interrelating solubility parameters with LSER molecular descriptors. The fundamental differences of the various approaches to hydrogen bonding interactions are discussed in an effort to explain incompatibilities and similarities. Simple QSPR-type expressions are proposed for fast solvent screening and related properties. Predictions of drug solubilities and wetting properties of solid surfaces are reported. The developments are made by having in mind their implementation in a thermodynamic equation-of-state framework for the reliable estimation of all basic thermodynamic quantities of compounds over a broad range of external conditions. The challenges and the perspectives of this unification are critically discussed.

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