

Thermochemistry of Substituted Benzamides and Substituted Benzoic Acids: Like Tree, Like Fruit?

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Abstract

© 2018 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim Structure–property analyses of thermodynamic properties in chemical families of R-substituted benzamides, R-substituted benzoic acids, as well as R-substituted benzenes have been performed. The general linear interrelations for the vaporization enthalpies and the gas-phase enthalpies of formation between the chemical families under study have been established. These linear correlations provide a simple method for prediction of thermodynamic properties for benzenes with various combination of R-group substituents on the benzene ring. In addition, the robust structure–property correlations revealed in this study can serve for the establishment of the internal consistency of experimental results available for each chemical series.

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Keywords

benzamides, combustion calorimetry, quantum chemistry, structure–property analysis, vapor pressure

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