

# Nearest-neighbor and non-nearest-neighbor interactions between substituents in the benzene ring. Experimental and theoretical study of functionally substituted benzamides

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## Abstract

© 2016 American Chemical Society. Standard molar enthalpies of formation of 2- and 4-hydroxybenzamides were measured by combustion calorimetry. Vapor pressures of benzamide and 2-hydroxybenzamide were derived by the transpiration method. Standard molar enthalpies of sublimation or vaporization of these compounds at 298 K were obtained from vapor pressure temperature dependence. Thermochemical data on benzamides with hydroxyl, methyl, methoxy, amino, and amide substituents were collected, evaluated, and tested for internal consistency. The high-level G4 quantum-chemical method was used for mutual validation of the experimental and theoretical gas-phase enthalpies of formation. Sets of nearest-neighbor and non-nearest-neighbor interactions between substituents in the benzene ring have been evaluated. A simple incremental procedure has been suggested for a quick appraisal of the vaporization and gas-phase formation enthalpies of the substituted benzamides. (Chemical Equation Presented).

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