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Benchmark Thermodynamic Properties of Methyl- and Methoxybenzamides: Comprehensive Experimental and Theoretical Study

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Abstract

© 2016 American Chemical Society.The enthalpies of formation of 2-, 3-, and 4-CH3-benzamide, as well as for 2-CH3O-benzamide, were measured by using combustion calorimetry. Vapor pressures of the isomeric CH3- and CH3O-benzamides were measured by using the transpiration method. The enthalpies of sublimation/vaporization of these compounds at 298 K were obtained from temperature dependencies of vapor pressures. The enthalpies of solution of the isomeric CH3- and CH3O-benzamides were measured with solution calorimetry. The enthalpies of sublimation of m- and p-substituted benzamides were independently derived with help of a solution calorimetry-based procedure. The enthalpies of fusion of the CH3-benzamides were derived from differential scanning calorimetry measurements. Thermochemical data on CH3- and CH3O-benzamides were collected, evaluated, and tested for internal consistency. A simple incremental procedure was suggested for a quick appraisal of vaporization enthalpies of substituted benzamides. The high-level G4 quantum-chemical method was used for mutual validation of the experimental and theoretical gas-phase enthalpies of formation. A remarkable ability of the G4-based atomization procedure to calculate reliable enthalpies of formation was established for the set of aliphatic and aromatic amides. An outlook for the proper validation of the G4-AT procedure was discussed.

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