Experimental and Computational Study on the Thermochemistry of Some Isomers of Bromoaniline

M.A.V. Ribeiro da Silva[C,S], A.I.M.C. Ferreira and J.R.B. Gomes
Centro de Investigação em Químic, Departamento de Químic, Faculdade de Ciências, Universidade do Porto, Porto, Portugal
risilva@fc.up.pt

The standard (p^o = 0.1 MPa) molar enthalpies of formation for solid or liquid and gaseous 2-bromoaniline, 3-bromoaniline, 4-bromoaniline, 2,4-dibromoaniline, 2,5-dibromoaniline, 2,6-dibromoaniline and 2,4,6-tribromaniline were derived from the standard molar enthalpies of combustion, in oxygen, at T = 298.15 K, measured by rotating-bomb calorimetry, and the standard molar enthalpies of sublimation or vaporization, at T = 298.15 K, measured by Calvet microcalorimetry. The standard molar enthalpies of formation for these compounds were determined by DFT calculations. The theoretical calculations were performed at the BP86/6-31 G* approach. Estimated values are in good agreement with the reported experimental ones. The results are discussed in terms of molecular structure.
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