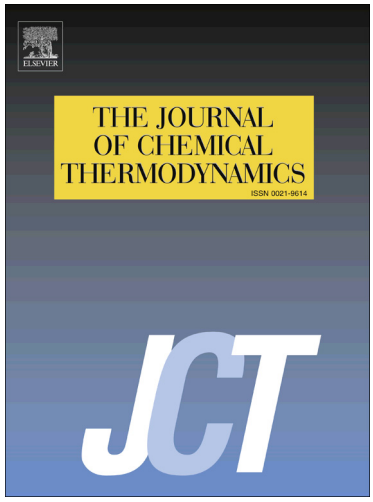

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Gas-phase enthalpies of formation of ethyl hydroxybenzoates: an experimental and theoretical approach

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Abstract

In this work, we report the molar enthalpies of formation of ethyl 2-, 3-, and 4-hydroxybenzoates in gas-phase at $T = 298.15$ K, derived from experimental techniques such as static-bomb combustion calorimetry, differential scanning calorimetry, and thermogravimetric analysis. We calculated as well the enthalpies of formation (of the same compound set) in gas-phase through the Gaussian G4 composite method, and a Boltzmann averaging procedure weighted with the Gibbs free energy. Finally, we discuss and compare experimental and theoretical results.

Keywords: Energy of Combustion; Enthalpy of Formation; Heat Capacity, Ethyl hydroxybenzoate; G4 Method.