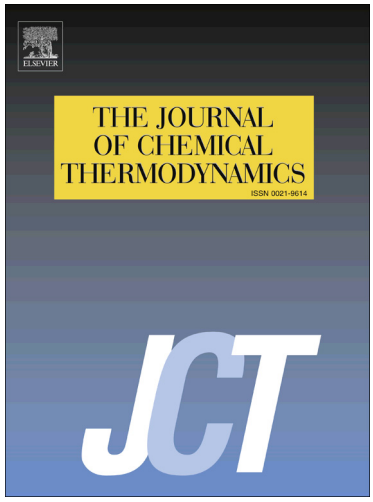

Experimental and theoretical study of methyl n-hydroxybenzoates

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PII: S0021-9614(18)30332-X
DOI: https://doi.org/10.1016/j.jct.2018.04.011
Reference: YJCHT 5388

To appear in: *J. Chem. Thermodynamics*

Received Date: 18 December 2017
Revised Date: 13 April 2018
Accepted Date: 16 April 2018

Please cite this article as: J.M. Ledo, H. Flores, J.M. Solano-Altamirano, F. Ramos, J.M. Hernández-Pérez, E.A. Camarillo, B. Rabell, M.P. Amador, Experimental and theoretical study of methyl n-hydroxybenzoates, *J. Chem. Thermodynamics* (2018), doi: https://doi.org/10.1016/j.jct.2018.04.011

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Abstract

We determined the standard molar enthalpies of formation in gas-phase, at T = 298.15 K, of the methyl 2-, 3-, and 4-hydroxybenzoates, through static bomb combustion calorimetry and thermogravimetry. The enthalpies of formation in gas phase were derived from experimental combustion energies and phase-change enthalpies. In addition, we calculated the enthalpies of formation in the gas-phase with the Gaussian G4 composite method combined with atomization reactions and a Boltzmann weighted average to account for the conformational diversity of each compound. Experimental and theoretical determinations differ by less than 2 kJ·mol^{-1}. We found that intramolecular hydrogen bonding strongly stabilizes methyl 2-hydroxybenzoate.

Keywords: Energy of Combustion; Enthalpy of Formation, Enthalpy of sublimation, methyl hydroxybenzoates, G4 composite method.

1. Introduction

Esters derived from benzoic acid have been widely studied in recent years [1-6]. In particular, our research group conducted a theoretical-experimental study of the ethyl 2-, 3-, and 4-hydroxybenzoates [7]. Furthermore, Almeida *et al.* recently published a thermochemical analysis, which included experimental measurements performed on methyl 4-hydroxybenzoate [5]. Our research group reported its sublimation enthalpy for this compound obtained by thermogravimetry as well [8]. The interest in these compounds emerges from their vast utilization in the food, cosmetic, and pharmaceutical industries as preservatives, because of their broad-spectrum antimicrobial properties. In addition, they serve as basic materials in the preparation of fragrances and flavourings [9-14].

In the present work, we report the thermochemical properties, obtained both theoretically and experimentally, of the methyl 2-, 3-, and 4-hydroxybenzoates. Hereon we will denote these