

Search for publications, researchers, or questions



or

Discover by

Join for free

Log in

See all >

26 References

Share

Request full-text

Energetics and structural properties of neutral and deprotonated phenyl carbinols

Article in *The Journal of Chemical Thermodynamics* 97 · February 2016 with 20 Reads

DOI: 10.1016/j.jct.2016.02.010



1st [Juan Z Dávalos](#)

39.52 · Institute of Physical Chemistry Rocasolano



2nd [Andrés Guerrero](#)

29.81 · University of California, Davis



3rd [Ana C. Valderrama-Negrón](#)

+ 1



Last [A. F. Lago](#)

29.62 · Universidade Federal do ABC (UFABC)

Show more authors

Abstract

Theoretical and experimental studies on the energetics, structure and other physicochemical properties of neutral 1-phenylethanol (1OH), diphenylmethanol (2OH) and triphenylmethanol (3OH) and their corresponding deprotonated anions (oxyanions, formed by deprotonation of the OH group) are reported in this work. The standard enthalpies of formation in the gas phase at 298.15 K, (g) have been determined. Quantum chemical calculations, at the DFT (particularly M05-2X method) and in some cases at the ab initio (G3) levels, have shed light on structural and electronic effects on the thermodynamic stability and intrinsic acidity of the studied compounds. These calculations confirmed the excellent consistency of the experimental results.

Do you want to **read the rest** of this article?

Request full-text

Citations 0

References 26

The impact of the Wenchuan earthquake on birth outcomes.

Article · Jan 1986

M COLOMINA Pilar Jiménez M.V. Roux C TURRION C TURRION

Read

Recommended Key Values for Thermodynamics

Article · Jan 1978 · *The Journal of Chemical Physics*