

A Thermodynamic Insight on the Structure and Energetics of 2,4,6-Triphenyl-1,3,5-Triazine

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2,4,6-triphenyl-1,3,5-triazine is an organic compound with interesting thermophysical and thermochemical properties. Its molecular unit is found in various applications in the fields of liquid crystals and non-linear optics, among others [1-3]. Therefore, we present a study of its thermodynamic properties, including vapor pressures, heat capacities and enthalpy of combustion of the solid, as well as fusion and sublimation enthalpies and entropies. In this work, the gas phase structure and energetics are also investigated, combining the experimental results with the results obtained by the MP2 and B3LYP theoretical methods. This work comprises the use of techniques like differential scanning calorimetry (DSC), a combined Knudsen/Quartz crystal method, Calvet microcalorimetry, and combustion calorimetry. The comparison of the results obtained in this work with similar ones presented in the literature for the analogous compound 1,3,5-triphenylbenzene brings out some interesting conclusions.

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