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Thermodynamic properties of 1,2-cyclohexanediols

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Abstract

© 2015 Pleiades Publishing, Ltd. The enthalpy values for the combustion and formation of crystalline cis and trans-1,2-cyclohexanediols are determined via bomb calorimetry. The vapor pressures of the compounds and their enthalpies of sublimation are measured. Using quantum-chemical methods, the reliability of the experimental data is estimated, the molecular structures of the compounds are studied, and the structures of the most stable conformers are established. The energy values of the intramolecular hydrogen bonds in the diol molecules are found.

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Keywords

1,2-cyclohexanediols, enthalpy of formation, enthalpy of sublimation, hydrogen bonds, quantum-chemical calculations