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Thermodynamic properties of 2-methyl lactic acid

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ABSTRACT

The measurements of the values of the enthalpy of formation, vaporisation, sublimation and fusion of 2-methyl lactic acid have been performed using methods of combustion calorimetry, transpiration method and differential scanning calorimetry. A conformational analysis has been conducted to identify a set of stable conformers of the compound. Methods of statistical thermodynamics have been used to calculate the thermodynamic functions of the acid in the ideal gas state considering the contribution of the internal rotation in “rigid rotator – anharmonic oscillator” approximation within temperature interval (298.15-1500) K for the conformers under study.

Key words: *lactic acid, combustion calorimetry, transpiration method, differential scanning calorimetry, vapour pressure, enthalpy of formation, thermodynamic functions, ab initio calculations, statistical thermodynamic.*

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