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Sublimation enthalpy of 1,3-thiazine structural analogues: experimental determination and estimation based on structural clusterization

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Highlights

- *Vapor pressures of 4 bioactive 1,3-thiazine and 1,3-selenazine derivatives have been measured*
- *Thermodynamic functions of sublimation have been calculated*
- *Melting temperatures and enthalpies were determined by DSC*
- *Sublimation enthalpies were calculated by using approach of structural clusterization*

ABSTRACT

The saturated vapor pressures of 4 nonaromatic bicyclic 1,3-thiazine and 1,3-selenazine derivatives have been measured by the method of transpiration by inert gas-carrier in the temperature range of 308-392 K. Based on the experimental data the thermodynamic functions of sublimation have been calculated. The sublimation enthalpies of the compounds vary from 104 to 150 kJ·mol⁻¹ depending on the chemical nature of the substituent in the aryl moiety and the heteroatom in the bicyclic fragment. The crystal lattice energy of thiazines

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