INFLUENCE OF MOLECULAR SYMMETRY ON THE ENERGY OF VAPORIZATION OF ETHYLENE GLYCOL ETHERS AND C_1–C_{10} ALCOHOLS

Emelyanov V.V., Elbakari A.V., Vostrikov S.V., Verevkin S.P.
Samara State Technical University
443100, Samara, Molodogvardeyskaya st., 244

Ethers of ethylene glycol and C_1-C_{10} alcohols of various structures have found wide application in modern high-tech industries: they are employed in absorption processes for the purification of natural gases from acidic impurities; they are used as components of hydraulic and brake fluids; and they serve as effective co-solvents and transdermal conductors in pharmaceuticals and cosmetology.

Such a wide range of applications for representatives of this series of compounds is due to their high thermodynamic stability and low volatility, as well as the possibility of varying other physicochemical properties through targeted modeling of the chemical structure when creating symmetrical or asymmetrical ethers.

The determining parameter for considering the applicability of ethylene glycol ethers in a particular area is the enthalpy of evaporation, on the basis of which it is possible to evaluate intermolecular interactions in organic liquids or thermodynamic compatibility with materials for various purposes.

The diversity of ethylene glycol ethers (both symmetrical and asymmetrical in nature) imposes experimental limitations on the determination of the enthalpy of vaporization values by direct or indirect methods (mass transfer, ebulliometry, etc.) due to the labor-intensive nature of the synthesis and isolation of compounds.

As alternative approaches in world practice, empirical correlation dependencies of the enthalpy of evaporation on chromatographic retention parameters or physical/structural quantities (boiling temperatures, enthalpies of solution, number of homologous elements, etc.) are used, as well as high-level quantum-chemical calculations based on gas-phase enthalpies of formation.

This paper validates available literature data on the enthalpies of vaporization of ethylene glycol ethers and C_1-C_{10} alcohols of varying structure and symmetry. Correlations between the enthalpies of vaporization and the above-mentioned arguments (in the form of structural or thermophysical parameters) are demonstrated for a wide range of ethers. The obtained values are compared with those obtained through quantum-chemical calculations. An array of enthalpy of vaporization values is proposed and substantiated for a number of the ethers considered.

Acknowledgments: This work was supported by the Ministry of Science and Higher Education of the Russian Federation (theme № FSSE-2025-0006) as part of the state task of the Samara State Technical University.