DETERMINATION OF VAPOR PRESSURE AND ENTHALPY OF VAPORIZATION OF NEOPENTYL GLYCOL ESTERS OF FATTY CARBOXYLIC ACIDS

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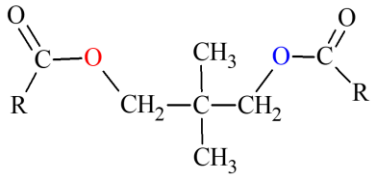
Esters based on fatty acids and neopentyl glycol (NPG) are used as base oils and can also serve as one of the components of synthetic lubricants.

In this work, a series of esters of neopentyl glycol and octanoic, 2-ethylhexanoic, decanoic, and dodecanoic acids was synthesized (see Figure).



Structure of Neopentyl Glycole Diesters

Esters of neopentyl glycol and fatty acids of the C_8-C_{12} series were obtained by esterification in a self-catalytic mode in the presence of a solvent *n*-decane. The purity of the samples was determined by gas chromatography. The purity of the samples was more than 98% by weight. The values of sorption enthalpies, vapor pressures, and evaporation enthalpies were determined for the obtained samples.

The value of the change in internal energy $\Delta_{sorp}\bar{U}$ (kJ/mol) and sorption enthalpy $\Delta_{sorp}H$ (kJ/mol) at an experimental temperature was determined from the dependencies:

$$\ln(k/T) = C - \frac{\Delta_{sorp}\bar{U}}{RT}\ ;\ \Delta_{sorp}H = \Delta_{sorp}\bar{U} - RT \text{ and } k = \frac{t_R - t_M}{t_M},$$

where t_R– adjusted retention time of the esters, min; t_M - retention time of nonsorbing substance (*n*-hexane), min.

The vapor pressures of NPG esters were determined by the transpiration method. The obtained *p*-*T*-dependences were described by the equation of the form:

$$R \ln\left(\frac{P}{P_{aw}}\right) = A_f - \frac{B_f}{T} + \Delta^n_{ж}Cp^0 \ln\left(\frac{T}{T_{aw}}\right),$$

where P – is the vapor pressure at T; P_{aw} – is the vapor pressure at the average temperature of the study T_{aw}; A_f and B_f are empirical coefficients obtained by processing *p*-*T* data by the least squares method; $\Delta^n_{ж}Cp^0$ – the difference between the molar heat capacities of the gas and liquid phases [1].

$$\Delta_{vap}H^0_m(298{,}2) = -B_f + 298.2\ \Delta^n_{ж}Cp^0.$$

1. E. L. Krasnykh and S. V. Portnova. Journal of Structural Chemistry. 2017, 58, 4, 706

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