Method for calculation of thermal conductivity of hydrofluorochloro olefin isomers on the saturation line

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The problem of predicting the thermal conductivity of liquid cisisomers and trans-isomers of hydrochlorofluoroolefins on the coexistence curve is considered. The approach is based on linear correlation [1]:

$$\lambda_s^{(1)} = \lambda_0^{(1)} (a_1 + b_1 T_{\rm rb}^{(1)}), \tag{1}$$

where a_1 , b_1 are constant coefficients, $T_{\rm rb}^{(1)} = T/T_b^{(1)}$; T_b is the normal boiling point, K; $\lambda_0^{(1)} = p_c^{2/3} M^{-1/2} T_c^{-1/7} G u^{-4} + 0.05 \omega^4$; p_c and T_c are the critical pressure and the critical temperature; M is the molar mass, $Gu = T_c/T_b$, ω is the acentric factor.

If $\lambda_s^{(2)}$ of the cis-isomer is described by (1), then $\lambda_s^{(1)}$ of the transisomer is calculated by the formula:

$$\lambda_s^{(2)} = \lambda_0^{(1)} (a_1 \Gamma^\alpha + b_1 T_{\rm rb}^{(2)}), \tag{2}$$

where $\Gamma=T_b^{(2)}/T_b^{(1)};\ T_{\rm rb}^{(2)}=T/T_b^{(2)};\ T_b^{(1)},\ \lambda_b^{(1)}$ and $T_b^{(2)},\ \lambda_0^{(2)}$ are the characteristics of the trans-isomer and cis-isomer, respectively; $\alpha=0.15.$

The procedure was tested on the example of cis-isomers R1234ze(Z), R1336mzz(Z) and trans-isomers R1234ze(E), R1336mzz(E). Based on this method, λ_s of the cis-isomer R1132(Z) was predicted. This method was compared with known correlation models [1–3].

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^[2] Yang S, Tian J and Jiang H 2020 Fluid Phase Equilib. 509 112459

^[3] Kudryavtseva I V and Rykov S V 2022 Russ. J. Phys. Chem. A 96 2098–2104