

Development of Vapor-Pressure Correlations using Trouton's Rule

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Accurate predictive vapor-pressure correlations using only one or two input quantities are needed for applied thermodynamics. Such a correlation would be useful to describe the vapor pressure of petroleum fractions, since a normal boiling point and limited characterization (e.g., specific gravity) may be the only pseudocomponent information available. These correlations would be helpful for new compounds where only one or two vapor-pressure measurements may be available. Finally, simple correlations help understand the broad patterns of the vapor pressures of chemical compounds. Trouton's rule (1884) states that the ratio of the enthalpy of vaporization and the temperature at the normal boiling point is a constant for all substances, $\Delta H_{\text{vap}}/R.T_b = 10.5$. We have extended this simple and useful correlation, known here as Modified Trouton's Rule, which applies to most nonpolar and slightly polar substances, $\Delta H_{\text{vap}}/R.T_b = 8.85 + 0.006T_{\text{boil}}$. We have developed a universal correlation for vapor pressure, based upon two input quantities, T_{boil} and $\Delta H_{\text{vap},b}$, which is applicable to an intermediate pressure range (about 0.1 mmHg to the critical point). The one-parameter version of the correlation, where the enthalpy of vaporization is predicted using the Modified Trouton's Rule, provides a surprisingly accurate model for most nonpolar and slightly polar fluids. This indicates that the vapor pressure of this large fraction of all substances may be established to good accuracy by a single data point, and implies that the vapor pressures of nonpolar and slightly polar substances rarely cross. The two-parameter version of the correlation (where the experimental enthalpy of vaporization is also used) is needed for polar compounds, and provides an accurate predictive model for polar substances like water, ethanol and propanol. We conclude that the vapor pressure of chemical compounds falls into a simpler pattern than has previously been recognized.