Vapor-Liquid Equilíbrium Data for 2-propanol + 2-methyl-1-propanol + 3-methyl-1-butanol at 560 mmHg and 760 mmHg

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Higher alcohols are produced during bioethanol fermentation by transformations of amino acids. They are alcohols with number of carbon atoms between three and five, such as propyl alcohol, amyl alcohol and their isomers, and they are responsible for the odor of spirits. They are present in the fusel oil, a less volatile alcoholic fraction obtained during ethanol distillation. Although fusel oil is one of the main by-products of alcohol distillation, it is not properly harnessed by industries. Vapor-Liquid Equilibrium (VLE) data are essential for the knowledge of phase behavior and for obtaining parameters of thermodynamic models in order to describe or predict phase equilibrium. These models permit the correct calculation of phase equilibrium, an important step in the design and optimization of separation processes by computational simulation. This work aimed to study the VLE of these components. The ternary system studied was composed of 2-propanol, 2-methyl-1-propanol and 3-methyl-1-butanol at constant pressures of 560 mmHg and 760 mmHg. The VLE experiments were conducted in a FISCHER Ebuliometer (VLE 602). For each experimental point, after the system reach the VLE conditions (20 until 40 minutes), the temperature and pressure were measured and liquid and condensed vapor phases were collected, simultaneously These samples were later analyzed by gas chromatography for determining the compositions. Another contribution of this work was the binary interaction parameters obtained by adjusting the activity coefficient models (Wilson, NRTL and UNIQUAC) to the experimental data. The Aspen Plus simulator was used to adjust the parameters. The models proved to be adequate for representing the VLE of the studied system, and the temperature and vapor composition deviations between experimental and calculated data were low for all the models used.

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