

# Total Vapor Pressure Measurements for Heptane + 1-Pentanol, + 2-Pentanol, + 3-Pentanol, + 2-Methyl-1-butanol, + 2-Methyl-2-butanol, + 3-Methyl-1-butanol, and + 3-Methyl-2-butanol at 313.15 K

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Total vapor pressure measurements at 313.15 K are reported for binary systems of heptane with each of seven pentanol isomers: 1-pentanol, 2-pentanol, 3-pentanol, 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-1-butanol, and 3-methyl-2-butanol. The results were obtained using a Van Ness type apparatus and were fitted to the modified Margules equation using Barker's method. The four-parameter modified Margules equation represents the data to within an average absolute deviation of approximately 0.03 kPa.

## Introduction

In a previous study (Barton et al., 1996), total pressure measurements for binary mixtures of methanol with seven pentanol isomers were reported. The purpose of that work was to obtain data that would be useful in studying the effect of isomer structure on cross-association between different alcohol molecules.

When applied to binary mixtures of alcohols, most association models require values for the self-association constants of each alcohol in addition to the cross-association constant. Rather than try to obtain all three association constants from a binary alcohol + alcohol isotherm, it is better to obtain the self-association constants from other data; specifically from binary data for each alcohol mixed with a nonpolar diluent. These self-association constants may then be specified apriori in the fit of the association model to the binary alcohol + alcohol mixture leaving only the value of the cross-association constant to be determined from that data.

The purpose of the present study was to obtain data that would allow the determination of the self-association constants for the pentanol isomers. To this end, vapor–liquid equilibrium data at 313.15 K are presented here for mixtures of heptane with each of seven isomers of pentanol.

Several sets of vapor–liquid equilibrium data have been reported previously for these systems. Isothermal results for heptane + 1-pentanol are available at 313.15 K (Zielkiewicz, 1994), 348.15 K (Trinh et al., 1972), 363.27 and 373.32 K (Treszczanowicz and Treszczanowicz, 1979), and at 348.15, 358.15, and 368.15 K (Machova et al., 1988). Other systems for which isothermal VLE have been published include heptane + 2-pentanol and heptane + 2-methyl-1-butanol (Wolfova et al., 1991), heptane + 3-methyl-1-butanol (Machova et al., 1988), and heptane + 3-pentanol (Wolfova et al., 1990), all at 348.15, 358.15, and 368.15 K. In addition, Wolfova et al. (1990) also reported data for heptane + 2-methyl-2-butanol at 328.15, 338.15, and 348.15 K.

## Experimental Section

**Apparatus and Procedure.** The apparatus is essentially the same as described in detail by Bhethanabotla

and Campbell (1991). It is of the Van Ness type (Gibbs and Van Ness, 1972) in which total pressure is measured as a function of overall composition in the equilibrium cell. Two modifications to the apparatus described by Bhethanabotla and Campbell have been made: the pressure gauge has been replaced with one of 0.001 kPa resolution as described by Pradhan et al. (1993) and the piston injectors have been replaced with Ruska pumps (model 2200) having a resolution of 0.001 cm<sup>3</sup>.

The overall composition in the equilibrium cell is changed by charging metered amounts of the pure components from their respective piston injectors. The pressure in the cell is read after equilibration. The small correction (less than 0.001 in mole fraction) to convert the overall mole fraction in the equilibrium cell to the liquid phase mole fraction is made as part of the data reduction procedure as described by Bhethanabotla and Campbell.

Experimental uncertainties are  $\pm 0.1\%$  in pressure,  $\pm 0.02$  K in temperature, and between  $\pm 0.0005$  and  $\pm 0.001$  in mole fraction, the smaller value applying at the extremes in composition.

**Materials.** All chemicals were obtained from Aldrich and had percent purities (by chromatographic analysis, as given by the manufacturer) of 99.7 (1-pentanol), 99.3 (2-pentanol), 99.7 (3-pentanol), 99.9 (2-methyl-1-butanol), 99.5 (2-methyl-2-butanol), 99.9 (3-methyl-1-butanol), 99.6 (3-methyl-2-butanol), and 99.2 (heptane). A different lot of heptane (99.7% purity) was used for the heptane + 1-pentanol run. All chemicals were degassed by vacuum distillation and were used without additional purification. The pure component vapor pressures measured in this study are reported in Table 1 where they are compared to the values reported by Butler et al. (1935), Thomas and Meatyard (1963), Ambrose and Sprake (1970), and Barton et al. (1996) and with the compilations of Ambrose and Walton (1989) and the Thermodynamic Research Center (1996). Generally, good agreement is found between the reported results and those of the present study. The six vapor pressures measured for the same lot of heptane agree to within  $\pm 0.025$  kPa, which is at the limit of experimental uncertainty. The vapor pressure of heptane from the heptane + 1-pentanol run was slightly higher (0.09 kPa) than the average of the other six determinations.

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