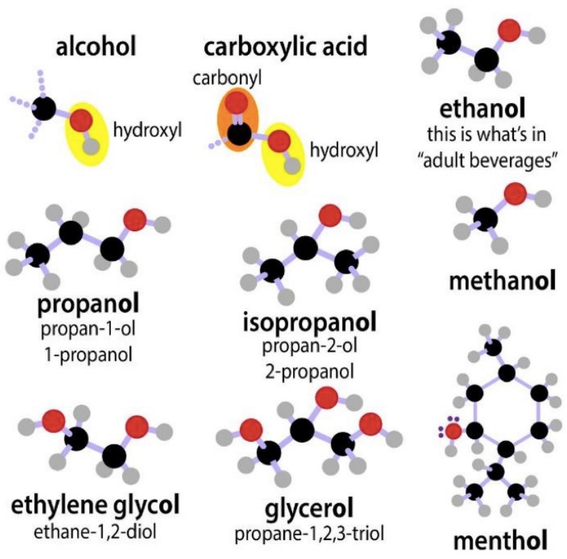
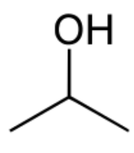
RAMSAY- YOUNG METHOD

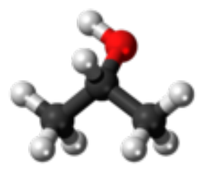
Vapor-Liquid Equilibrium of Alcohols | Isomerization effect

Alcohols: *n-iso* effect



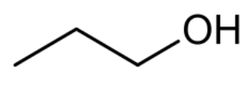
Hazards	
Occupational safety and health (OHS/OSH):	
Main hazards	Flammable, mildly toxic[6]
GHS labelling:	
Pictograms	
Signal word	**Danger**
Hazard statements	H225, H302, H319, H336
Precautionary statements	P210, P261, P305+P351+P338
NFPA 704 (fire diamond)	
Flash point	Open cup: 11.7 °C (53.1 °F; 284.8 K) Closed cup: 13 °C (55 °F)
Autoignition temperature	399 °C (750 °F; 672 K)
Explosive limits	2–12.7%
Threshold limit value (TLV)	980 mg/m³ (TWA), 1225 mg/m³ (STEL)
Lethal dose or concentration (LD, LC):	
LD_{50} (median dose)	12800 mg/kg (dermal, rabbit)[8] 3600 mg/kg (oral, mouse) 5000 mg/kg (oral, rat)[8] 2364 mg/kg (oral, rabbit)
LC_{50} (median concentration)	53,000 mg/m³ (inhalation, mouse)[citation needed] 12,000 ppm (rat, 8 h)[8]
LC_{Lo} (lowest published)	16,000 ppm (rat, 4 h) 12,800 ppm (mouse, 3 h)[8]
NIOSH (US health exposure limits):	
PEL (Permissible)	TWA 400 ppm (980 mg/m³)[7]
REL (Recommended)	TWA 400 ppm (980 mg/m³), ST 500 ppm (1225 mg/m³)[7]
IDLH (Immediate danger)	2000 ppm[7]

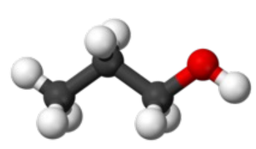




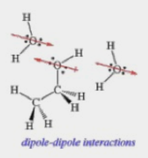
2-propanol
isopropanol

Hazards	
Occupational safety and health (OHS/OSH):	
Main hazards	Flammable liquid
GHS labelling:	
Pictograms	
Signal word	**Danger**
Hazard statements	H225, H302, H318, H336
Precautionary statements	P210, P261, P280, P305+P351+P338
NFPA 704 (fire diamond)	
Flash point	22 °C (72 °F; 295 K)
Autoignition temperature	371 °C (700 °F; 644 K)
Explosive limits	2.2–13.7%[2]
Lethal dose or concentration (LD, LC):	
LD_{50} (median dose)	2800 mg/kg (rabbit, oral) 1699 mg/kg (mouse, oral)[4] 1870 mg/kg (rat, oral)[5]
NIOSH (US health exposure limits):	
PEL (Permissible)	TWA 200 ppm (500 mg/m³)[2]
REL (Recommended)	TWA 200 ppm (500 mg/m³) ST 250 ppm (625 mg/m³) [skin][2]
IDLH (Immediate danger)	800 ppm[2]

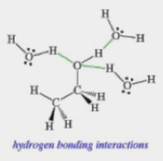




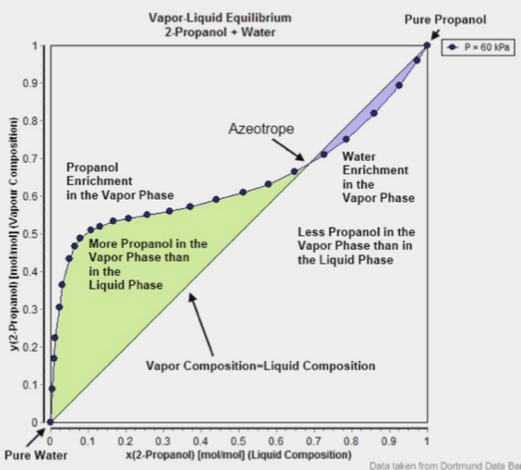
1-propanol
propanol



dipole-dipole interactions

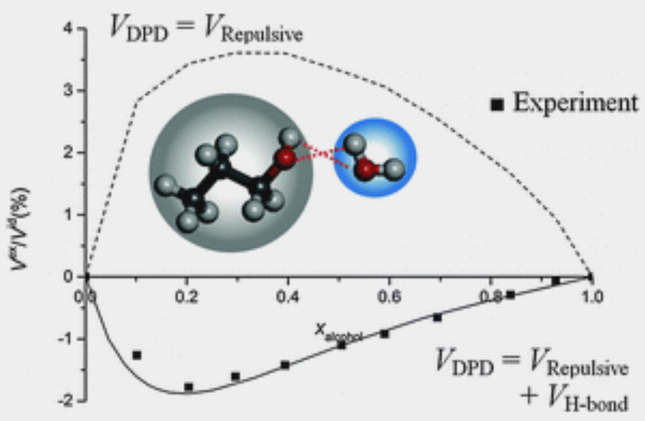


hydrogen bonding interactions



Water to 1-propanol

Fractional volume changes



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Phase Equilibria of Alcohols in

Mixtures with n-Alkanes and Water

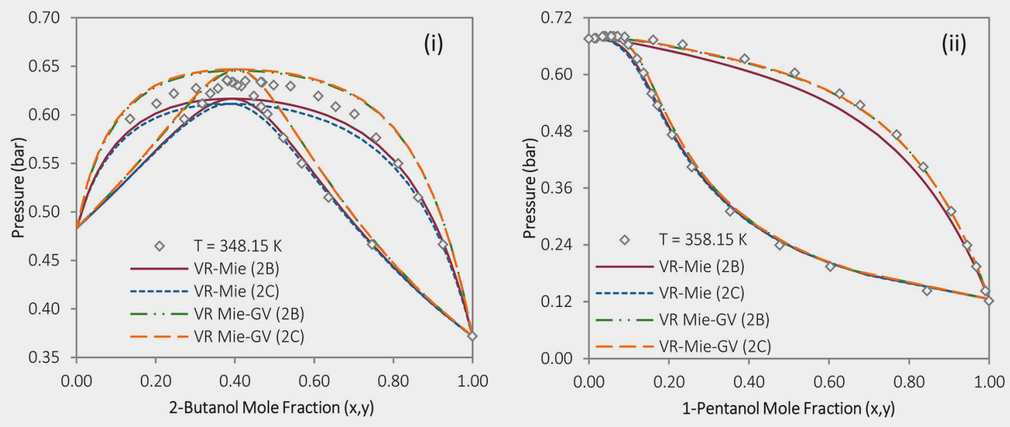

Figure 5. Comparison of polar and nonpolar SAFT-VR Mie parameter sets applied to alcohol/*n*-alkane mixtures: (i) 2-butanol/*n*-heptane at 348.15 K (63) and (ii) 1-pentanol/*n*-heptane at 358.15 K.

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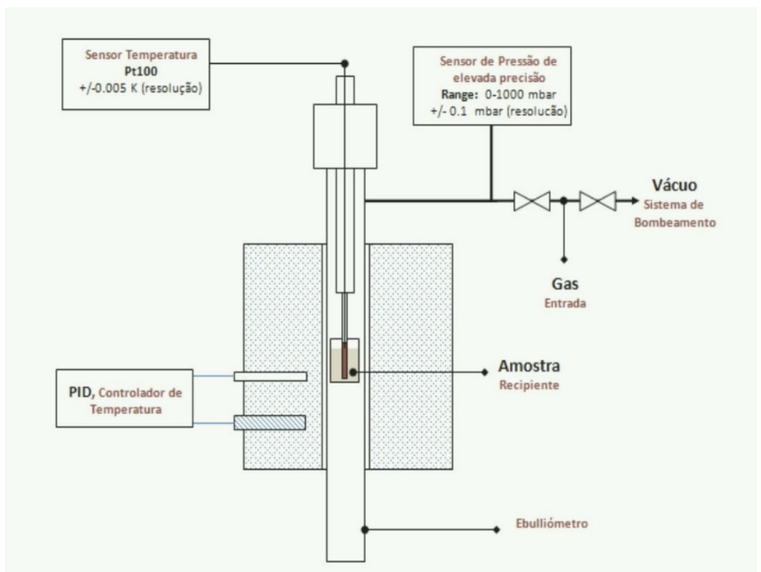
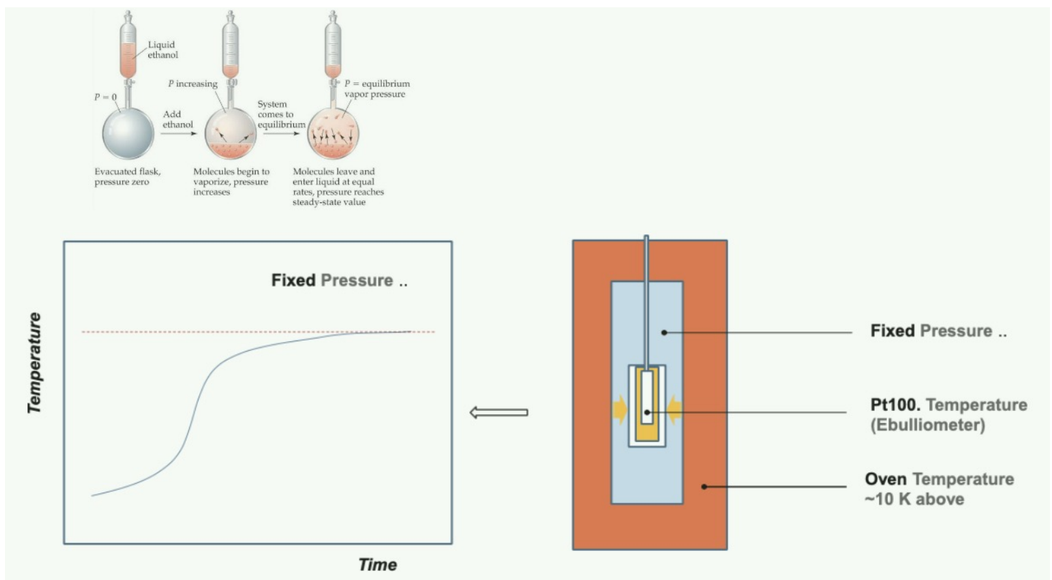
Methodology & Strategy

Vapor Pressure Measurements



Microebuliometer



Results & Comments:

Vapor Pressure *vs.* Temperature

$$\mu\,(\mathrm{cr,l};p;T) = \mu\,(\mathrm{g};p;T)$$

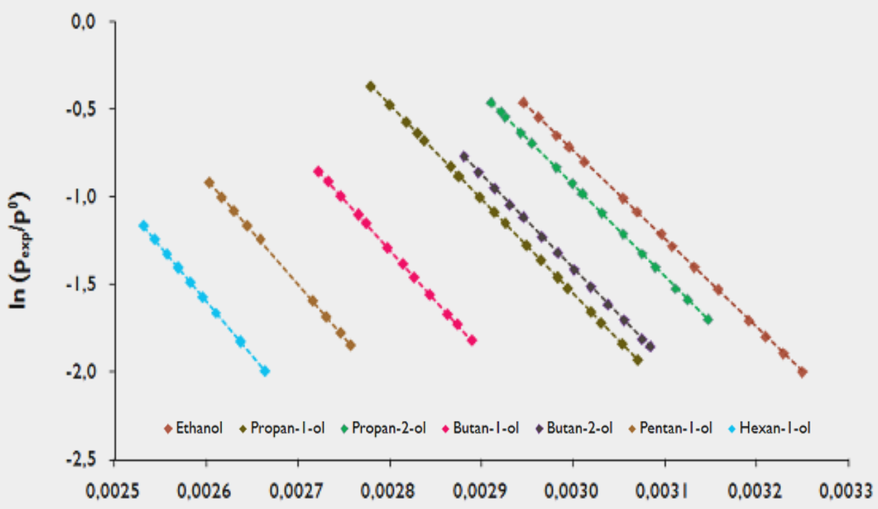
Two phases (α and β) in equilibrium at constant pressure and temperature have the same Gibbs free energy:

$$G_\alpha = G_\beta$$

Recalling that $dG = VdP - SdT$ yields:

$$V_\alpha\,dP - S_a\,dT = V_\beta\,dP - S_\beta\,dT$$

or $$dP/dT = (V_\beta - V_\alpha)/(S_\beta - S_\alpha) = \Delta S/\Delta V$$



Alcohol	m (K)	b	R^2
Ethanol	-5032 ± 5	14.36 ± 0.02	0.999986
Propan-1-ol	-5384 ± 4	14.60 ± 0.01	0.999992
Propan-2-ol	-5235 ± 3	14.77 ± 0.01	0.999996
Butan-1-ol	-5765 ± 9	14.84 ± 0.02	0.999976
Butan-2-ol	-5341 ± 8	14.61 ± 0.02	0.999974
Pentan-1-ol	-6009 ± 15	14.72 ± 0.04	0.999956
Hexan-1-ol	-6267 ± 16	14.69 ± 0.04	0.999955

Clausius-Clapeyron equation

$$\frac{\mathrm{d}\ln(p)}{\mathrm{d}T} = \frac{\Delta^{\mathrm{g}}_{\mathrm{cr,l}} H_m}{R\,T^2} \qquad pV = nRT$$

$$\ln\frac{p}{p^0} = -m\left(\frac{1}{T}\right) + b$$

Clarke & Glew Equation

$$R\ln\left(\frac{p}{p^0}\right) = -\Delta^{\mathrm{g}}_{\mathrm{cr,l}}G^0_{\mathrm{m}}(\theta) + \Delta^{\mathrm{g}}_{\mathrm{cr,l}}H^0_{\mathrm{m}}(\theta)\left(\frac{1}{\theta} - \frac{1}{T}\right) + \Delta^{\mathrm{g}}_{\mathrm{cr,l}}C^0_{p,\mathrm{m}}(\theta)\left(\frac{\theta}{T} - 1 + \ln\left(\frac{T}{\theta}\right)\right)$$

Propan-1-ol

Phase behavior	
Triple point	148.75 K (–124.4 °C), ? Pa
Critical point	536.9 K (263.8 °C), 5200 kPa
Std enthalpy change of fusion, $\Delta_{fus}H^\ominus$	5.37 kJ/mol
Std entropy change of fusion, $\Delta_{fus}S^\ominus$	36 J/(mol·K)
Std enthalpy change of vaporization, $\Delta_{vap}H^\ominus$	47.5 kJ/mol
Std entropy change of vaporization, $\Delta_{vap}S^\ominus$	126.6 J/(mol·K)

Propan-2-ol

Phase behavior	
Triple point	184.9 K (–88.2 °C), ? Pa
Critical point	508.7 K (235.6 °C), 5370 kPa
Std enthalpy change of fusion, $\Delta_{fus}H^\ominus$	5.28 kJ/mol
Std entropy change of fusion, $\Delta_{fus}S^\ominus$	28.6 J/(mol·K)
Std enthalpy change of vaporization, $\Delta_{vap}H^\ominus$	44.0 kJ/mol
Std entropy change of vaporization, $\Delta_{vap}S^\ominus$	124 J/(mol·K)

1. The volatility of the alcohols studied can be ordered:

   Etanol > Propan-2-ol > Propan-1-ol > Butan-1-ol > Butan-2-ol > Pentan-1-ol > Hexan-1-ol

2. Higher number of carbon atoms (methylene, $-CH_2-$) leads to less volatility & higher enthalpy of vaporization;
3. The isomerization strongly effects the volatility.

NIST Chemistry WebBook https://webbook.nist.gov/chemistry/
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