

Activity Coefficients at Infinite Dilution of Organic Solutes and Water
in Tributylethylphosphonium Diethylphosphate Using Gas – Liquid
Chromatography. Thermodynamic Properties of Mixtures Containing
Ionic Liquids.

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Table 1S. The sources and mass fraction purities of materials used.^a

Chemical name ^a	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
[P _{2,4,4,4}][DEP]	Iolitec	0.95	373 K, Vacuum Drying Ovens, 48h	-	-
Pentane	Fluka	≥ 0.99	—	—	—
Hexane	Fluka	≥ 0.99	—	—	—
3-Methylpentane	Aldrich	≥ 0.99	—	—	—
2,2-Dimethylbutane	Aldrich	≥ 0.99	—	—	—
Heptane	Aldrich	≥ 0.995	—	—	—
Octane	Aldrich	≥ 0.99	—	—	—
2,2,4-Trimethylpentane	Aldrich	≥ 0.99	—	—	—
Nonane	Aldrich	≥ 0.99	—	—	—
Decane	Aldrich	≥ 0.99	—	—	—
Cyclopentane	Aldrich	≥ 0.99	—	—	—
Cyclohexane	Aldrich	≥ 0.99	—	—	—
Methylcyclohexane	Aldrich	≥ 0.99	—	—	—
Cycloheptane	Aldrich	≥ 0.98	—	—	—
Cyclooctane	Fluka	≥ 0.99	—	—	—
Pent-1-ene	Acros	≥ 0.985	—	—	—
Hex-1-ene	Aldrich	≥ 0.99	—	—	—
Cyclohexene	Aldrich	≥ 0.99	—	—	—
Hept-1-ene	Aldrich	≥ 0.99	—	—	—
Oct-1-ene	Aldrich	≥ 0.98	—	—	—
Dec-1-ene	Aldrich	≥ 0.97	—	—	—
Pen-1-yne	Aldrich	≥ 0.97	—	—	—
Hex-1-yne	Aldrich	≥ 0.97	—	—	—
Hept-1-yne	Aldrich	≥ 0.98	—	—	—
Oct-1-yne	Aldrich	≥ 0.97	—	—	—
Benzene	Aldrich	≥ 0.998	—	—	—
Toluene	Aldrich	≥ 0.998	—	—	—
Ethylbenzene	Aldrich	≥ 0.998	—	—	—
<i>o</i> -Xylene	Aldrich	≥ 0.99	—	—	—
<i>m</i> -Xylene	Aldrich	≥ 0.99	—	—	—
<i>p</i> -Xylene	Aldrich	≥ 0.99	—	—	—
Styrene	Aldrich	≥ 0.999	—	—	—
Methanol	Aldrich	≥ 0.999	—	—	—
Ethanol	Aldrich	≥ 0.998	—	—	—
Water	own source	—	distillation, filtration	≥ 0.999	density
Thiophene	Aldrich	≥ 0.99	—	—	—
Oxolane (Tetrahydrofurane, THF)	Aldrich	≥ 0.999	—	—	—
1,4-Dioxane	Aldrich	≥ 0.998	—	—	—
2-Methoxy-2-	Aldrich	≥ 0.998	—	—	—

Chemical name ^a	Source	Initial mass fraction purity	Purification method	Final mass fraction purity	Analysis method
methylpropane (<i>tert</i> -Butyl methyl ether)	Aldrich	≥ 0.99	–	–	–
2-Methoxy-2-methylbutane (Methyl <i>tert</i> -pentyl ether)	Aldrich	≥ 0.99	–	–	–
2-Ethoxy-2-methylpropane (Ethyl <i>tert</i> -butyl ether)	Aldrich	≥ 0.999	–	–	–
Ethoxyethane (Diethyl ether)	Aldrich	≥ 0.99	–	–	–
1-Propoxypropane (Di- <i>n</i> -propyl ether)	Fluka	≥ 0.99	–	–	–
2-Propan-2-yloxypropane (Di- <i>iso</i> -propyl ether)	Aldrich	≥ 0.993	–	–	–
1-Butoxybutane (Di- <i>n</i> -butyl ether)	Aldrich	≥ 0.999	–	–	–
Propan-2-one (Acetone)	Aldrich	≥ 0.99	–	–	–
Pentan-2-one	Aldrich	≥ 0.99	–	–	–
Pentan-3-one	Aldrich	≥ 0.99	–	–	–
Hexan-2-one	Aldrich	≥ 0.99	–	–	–
Hexan-3-one	Aldrich	≥ 0.99	–	–	–
Acetonitrile	Fluka	≥ 0.999	–	–	–
Pyridine	Aldrich	≥ 0.998	–	–	–
1-Nitropropane	Aldrich	≥ 0.985	–	–	–

^a Names in parentheses are common names used in the text.

Table 2S. Mean column pressure, \bar{p} , inlet column pressure, p_i , outlet column pressure, p_o and standard state of solutes at given temperatures, st. state^a

solute	T / K					
	328.15	338.15	348.15	358.15	368.15	
pentane	\bar{p} / kPa	112.5	112.7	109.7	110.5	110.5
	p_i / kPa	122.2	120.2	119.4	120.2	120.2
	p_o / kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
hexane	\bar{p} / kPa	112.5	112.7	109.7	110.5	110.5
	p_i / kPa	122.2	120.2	119.4	120.2	120.2
	p_o / kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
3-methylpentane	\bar{p} / kPa	112.5	112.7	109.7	110.5	110.5
	p_i / kPa	122.2	120.2	119.4	120.2	120.2
	p_o / kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
2,2-dimethylbutane	\bar{p} / kPa	112.5	112.7	109.7	110.5	110.5
	p_i / kPa	122.2	120.2	119.4	120.2	120.2
	p_o / kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
heptane	\bar{p} / kPa	112.5	112.7	109.7	110.5	110.5
	p_i / kPa	122.2	120.2	119.4	120.2	120.2
	p_o / kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
octane	\bar{p} / kPa	112.5	112.7	109.7	110.5	110.5
	p_i / kPa	122.2	120.2	119.4	120.2	120.2
	p_o / kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid

2,2,4-trimethylpentane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
nonane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
decane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
cyclopentane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
cyclohexane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
methylcyclohexane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
cycloheptane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid

		liquid	liquid	liquid	liquid	liquid
cyclooctane	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
1-pentene	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
1-hexene	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
cyclohexene	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
1-heptene	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
1-octene	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
1-decene	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid

1-pentyne		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
1-hexyne		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
1-heptyne		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
1-octyne		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.5	112.7	109.7	110.5	110.5
	pi /kPa	122.2	120.2	119.4	120.2	120.2
	po /kPa	102.2	100.2	99.4	100.2	100.2
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
benzene		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	133.1	132.3	132.3	133.7	133.7
	pi /kPa	168.8	160.0	160.0	161.4	161.4
	po /kPa	100.8	100.0	100.0	101.4	101.4
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
toluene		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	133.1	132.3	132.3	133.7	133.7
	pi /kPa	168.8	160.0	160.0	161.4	161.4
	po /kPa	100.8	100.0	100.0	101.4	101.4
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
ethylbenzene		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	133.1	132.3	132.3	133.7	133.7
	pi /kPa	168.8	160.0	160.0	161.4	161.4
	po /kPa	100.8	100.0	100.0	101.4	101.4
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	

		liquid	liquid	liquid	liquid	liquid
<i>o</i> -xylene	\bar{p} /kPa	133.1	132.3	132.3	133.7	133.7
	pi /kPa	168.8	160.0	160.0	161.4	161.4
	po /kPa	100.8	100.0	100.0	101.4	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
<i>m</i> -xylene	\bar{p} /kPa	133.1	132.3	132.3	133.7	133.7
	pi /kPa	168.8	160.0	160.0	161.4	161.4
	po /kPa	100.8	100.0	100.0	101.4	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
<i>p</i> -xylene	\bar{p} /kPa	133.1	132.3	132.3	133.7	133.7
	pi /kPa	168.8	160.0	160.0	161.4	161.4
	po /kPa	100.8	100.0	100.0	101.4	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
styrene	\bar{p} /kPa	133.1	132.3	132.3	133.7	133.7
	pi /kPa	168.8	160.0	160.0	161.4	161.4
	po /kPa	100.8	100.0	100.0	101.4	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
methanol	\bar{p} /kPa		133.0	132.3	132.3	133.7
	pi /kPa		167.7	160.0	160.0	161.4
	po /kPa		100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
ethanol	\bar{p} /kPa		133.0	132.3	132.3	133.7
	pi /kPa		160.7	160.0	160.0	161.4
	po /kPa		100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
water	\bar{p} /kPa	133.1	132.3	132.3	132.3	132.3
	pi /kPa	160.8	160.0	160.0	160.0	160.0
	po /kPa	100.8	100.0	100.0	100.0	100.0
	st. state	hypothetical	hypothetical	hypothetical	hypothetical	hypothetical

thiophene		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	133.1	132.3	132.3	132.3	133.7
	pi /kPa	160.8	160.0	160.0	160.0	161.4
	po /kPa	100.8	100.0	100.0	100.0	101.4
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
tetrahydrofuran		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	133.1	133.0	132.3	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
1,4-dioxane		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	133.1	133.0	132.3	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
methyl <i>tert</i> -butyl ether		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.5	112.1	109.7	110.5	110.5
	pi /kPa	122.2	121.8	119.4	120.2	120.2
	po /kPa	102.2	101.8	99.4	100.2	100.2
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
ethyl <i>tert</i> -butyl ether		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.3	112.4	109.7	110.5	110.5
	pi /kPa	122.0	121.8	119.4	120.2	120.2
	po /kPa	102.0	101.8	99.4	100.2	100.2
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
methyl <i>tert</i> -pentyl ether		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.3	112.1	109.7	110.5	110.5
	pi /kPa	122.0	121.8	119.4	120.2	120.2
	po /kPa	102.0	101.8	99.4	100.2	100.2
st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	
diethyl ether		liquid	liquid	liquid	liquid	liquid
	\bar{p} /kPa	112.5	112.1	109.7	110.5	110.5
	pi /kPa	122.2	121.8	119.4	120.2	120.2

	po /kPa	102.2	101.8	99.4	100.2	100.2
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
di- <i>n</i> -propyl ether	\bar{p} /kPa	110.7	111.1	111.1	111.2	111.2
	pi /kPa	120.4	120.8	120.8	120.9	120.9
	po /kPa	100.4	100.8	100.8	100.9	100.9
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
di- <i>iso</i> -propyl ether	\bar{p} /kPa	110.7	111.1	111.1	111.0	111.2
	pi /kPa	120.4	120.8	120.8	120.7	120.9
	po /kPa	100.4	100.8	100.8	100.7	100.9
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
di- <i>n</i> -butyl ether	\bar{p} /kPa	110.7	111.1	111.1	111.0	111.2
	pi /kPa	120.4	120.8	120.8	120.7	120.9
	po /kPa	100.4	100.8	100.8	100.7	100.9
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
acetone	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
2-pentanone	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
3-pentanone	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
2-haxanone	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4

	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
3-hexanone	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
acetonitrile	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
pyridine	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid
1-nitropropane	\bar{p} /kPa	133.1	133.0	132.2	132.3	133.7
	pi /kPa	160.8	160.7	160.0	160.0	161.4
	po /kPa	100.8	100.7	100.0	100.0	101.4
	st. state	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid	hypothetical liquid

^a Standard uncertainties u are $u(T) = 0.02$ K, $u(\bar{p}) = 0.06$ kPa, $u(p_i) = 0.1$ kPa, $u(p_o) = 0.07$ kPa

Figure 1S. DSC diagram for pure [P₂₄₄₄][DEP]

