2-Furanmethanol, tetrahydro-

Other names: 2-(hydroxymethyl)tetrahydrofuran
2-HYDROXYMETHYL-TETRAHYDROFURAN
2-oxolanemethanol
2-tetrahydrofurylmethanol
Furfuryl alcohol, tetrahydro-
NSC 15434
Oxolan-2-methanol
QO THFA
TETRAHYDRO-2-FURANCARBINOL
TETRAHYDROFURFURYL ALCOHOL
THFA
Tetrahydro-2-furanmethanol
Tetrahydro-2-furanylmethanol
Tetrahydro-2-furfuryl alcohol
Tetrahydro-2-furylmethanol
Tetrahydrofurfurylalkohol
Tetrahydrofuryl carbinol
Tetrahydrofurylalkohol
Tetrahydrofurylmethanol
«alpha»-Tetrahydrofurfuryl alcohol
Â«alphaÂ»-Tetrahydrofurfuryl alcohol

Inchi: InChI=1S/C5H10O2/c6-4-5-2-1-3-7-5/h5-6H,1-4H2

InchiKey: BSYVTEYKTMYBMK-UHFFFAOYSA-N

Formula: C5H10O2

SMILES: OCC1CCCO1

Mol. weight [g/mol]: 102.13

CAS: 97-99-4

Physical Properties

Property code	Value	Unit	Source
gf	-195.17	kJ/mol	Joback Method
hf	-369.00 ± 6.30	kJ/mol	NIST Webbook
hfl	-435.60 ± 5.90	kJ/mol	NIST Webbook
hfus	14.71	kJ/mol	Joback Method
hvap	66.60	kJ/mol	NIST Webbook
hvap	67.00 ± 2.00	kJ/mol	NIST Webbook

log10ws	-0.27		Crippen Method
logp	0.158		Crippen Method
mcvol	82.190	ml/mol	McGowan Method
pc	4856.20	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	853.00		NIST Webbook
ripol	1496.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1494.00		NIST Webbook
sl	219.20	J/mol×K	NIST Webbook
tb	451.00 ± 3.00	K	NIST Webbook
tb	451.20	K	NIST Webbook
tc	637.66	K	Joback Method
tf	330.00 ± 3.00	K	NIST Webbook
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.03	J/mol×K	606.08	Joback Method
cpg	207.41	J/mol×K	542.93	Joback Method
cpg	197.87	J/mol×K	511.36	Joback Method
cpg	187.81	J/mol×K	479.78	Joback Method
cpg	177.23	J/mol×K	448.21	Joback Method
cpg	216.46	J/mol×K	574.51	Joback Method
cpg	233.15	J/mol×K	637.66	Joback Method
cpl	190.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0436528	Pa×s	244.40	Joback Method
dvisc	0.0003221	Pa×s	448.21	Joback Method
dvisc	0.0005219	Pa×s	414.24	Joback Method
dvisc	0.0009219	Pa×s	380.27	Joback Method
dvisc	0.0018209	Pa×s	346.30	Joback Method
dvisc	0.0041702	Pa×s	312.34	Joback Method
dvisc	0.0116912	Pa×s	278.37	Joback Method
hvapt	46.50	kJ/mol	388.00	NIST Webbook
hvapt	46.20	kJ/mol	423.00	NIST Webbook

rfi	1.45250			293.20	Phase Equilibria for the Ternary Liquid Systems of (Water + Tetrahydrofurfuryl Alcohol + Cyclic Solvent) at 298.2 K
rhol	1050.75	kg/m3		298.15	Self-aggregation of liquids from biomass in aqueous solution

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.79248e+01
Coeff. B	-6.27566e+03
Coeff. C	1.99750e+01
Temperature range (K), min.	335.84
Temperature range (K), max.	477.57

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.92241e+01
Coeff. B	-9.24652e+03
Coeff. C	-1.07177e+01
Coeff. D	6.98190e-06
Temperature range (K), min.	193.00
Temperature range (K), max.	639.00

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid

283.15	100.00	1062.84
288.15	100.00	1058.59
293.15	100.00	1054.34
298.15	100.00	1050.06
303.15	100.00	1045.78
308.15	100.00	1041.48
313.15	100.00	1037.17
318.15	100.00	1032.83
323.15	100.00	1028.47
328.15	100.00	1024.08
333.15	100.00	1019.68
338.15	100.00	1015.24
283.15	2500.00	1064.37
288.15	2500.00	1060.15
293.15	2500.00	1055.94
298.15	2500.00	1051.72
303.15	2500.00	1047.47
308.15	2500.00	1043.19
313.15	2500.00	1038.92
318.15	2500.00	1034.57
323.15	2500.00	1030.3
328.15	2500.00	1025.88
333.15	2500.00	1021.52
338.15	2500.00	1017.04
283.15	5000.00	1065.68
288.15	5000.00	1061.47
293.15	5000.00	1057.3
298.15	5000.00	1053.11
303.15	5000.00	1048.9
308.15	5000.00	1044.66
313.15	5000.00	1040.41
318.15	5000.00	1036.11
323.15	5000.00	1031.87
328.15	5000.00	1027.49
333.15	5000.00	1023.18
338.15	5000.00	1018.75
283.15	7500.00	1066.97
288.15	7500.00	1062.8
293.15	7500.00	1058.64
298.15	7500.00	1054.48
303.15	7500.00	1050.31
308.15	7500.00	1046.09
313.15	7500.00	1041.89
318.15	7500.00	1037.62

323.15	7500.00	1033.41
328.15	7500.00	1029.13
333.15	7500.00	1024.84
338.15	7500.00	1020.45
283.15	10000.00	1068.24
288.15	10000.00	1064.09
293.15	10000.00	1060.0
298.15	10000.00	1055.84
303.15	10000.00	1051.69
308.15	10000.00	1047.48
313.15	10000.00	1043.41
318.15	10000.00	1039.11
323.15	10000.00	1034.93
328.15	10000.00	1030.63
333.15	10000.00	1026.39
338.15	10000.00	1022.06
283.15	20000.00	1073.16
288.15	20000.00	1069.11
293.15	20000.00	1065.1
298.15	20000.00	1061.08
303.15	20000.00	1057.06
308.15	20000.00	1052.96
313.15	20000.00	1048.93
318.15	20000.00	1044.81
323.15	20000.00	1040.79
328.15	20000.00	1036.6
333.15	20000.00	1032.49
338.15	20000.00	1028.31
283.15	30000.00	1077.84
288.15	30000.00	1073.88
293.15	30000.00	1069.97
298.15	30000.00	1066.04
303.15	30000.00	1062.11
308.15	30000.00	1058.12
313.15	30000.00	1054.21
318.15	30000.00	1050.15
323.15	30000.00	1046.28
328.15	30000.00	1042.2
333.15	30000.00	1038.22
338.15	30000.00	1034.16
283.15	40000.00	1082.28
288.15	40000.00	1078.41
293.15	40000.00	1074.62
298.15	40000.00	1070.75

303.15	40000.00	1066.94
308.15	40000.00	1063.05
313.15	40000.00	1059.19
318.15	40000.00	1055.24
323.15	40000.00	1051.44
328.15	40000.00	1047.5
333.15	40000.00	1043.64
338.15	40000.00	1039.68
283.15	50000.00	1086.55
288.15	50000.00	1082.72
293.15	50000.00	1078.97
298.15	50000.00	1075.22
303.15	50000.00	1071.49
308.15	50000.00	1067.61
313.15	50000.00	1063.91
318.15	50000.00	1060.12
323.15	50000.00	1056.41
328.15	50000.00	1052.52
333.15	50000.00	1048.73
338.15	50000.00	1044.89
283.15	60000.00	1090.57
288.15	60000.00	1086.83
293.15	60000.00	1083.18
298.15	60000.00	1079.49
303.15	60000.00	1075.79
308.15	60000.00	1072.09
313.15	60000.00	1068.44
318.15	60000.00	1064.68
323.15	60000.00	1061.07
328.15	60000.00	1057.3
333.15	60000.00	1053.6
338.15	60000.00	1049.83

Reference *https://www.doi.org/10.1021/je400783h*

Sources

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Thermophysical Properties of Furfural Compounds:	https://www.doi.org/10.1021/je400783h

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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Self-aggregation of liquids from biomass in aqueous solution:	https://www.doi.org/10.1016/j.jct.2013.06.020
Modeling Considerations:	https://en.wikipedia.org/wiki/Joback_method
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Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume