Furan, 2-methyl-

Other names:	2-Methylfuran
	2-Methylfurane
	2-methyloxole
	5-METHYLFURAN
	Methylfuran
	SILVAN
	Sylvan
	UN 2301
	«alpha»-Methylfuran
	Â«alphaÂ»-Methylfuran
Inchi:	InChI=1S/C5H6O/c1-5-3-2-4-6-5/h2-4H,1H3
InchiKey:	VQKFNUFAXTZWDK-UHFFFAOYSA-N
Formula:	C5H6O
SMILES:	Cc1ccco1
Mol. weight [g/mol]:	82.10
CAS:	534-22-5

Physical Properties

Property code	Value	Unit	Source
af	0.2700		KDB
affp	865.90	kJ/mol	NIST Webbook
basg	833.50	kJ/mol	NIST Webbook
dm	0.70	debye	KDB
hvap	32.20	kJ/mol	NIST Webbook
ie	8.38	eV	NIST Webbook
ie	8.37	eV	NIST Webbook
ie	8.31 ± 0.09	eV	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.37 ± 0.05	eV	NIST Webbook
ie	8.38 ± 0.01	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
ie	8.57	eV	NIST Webbook
ie	8.39 ± 0.01	eV	NIST Webbook
ie	8.39 ± 0.01	eV	NIST Webbook
log10ws	-5.68		Crippen Method
logp	1.588		Crippen Method
mcvol	67.720	ml/mol	McGowan Method

pc	4720.00 ± 103.40	kPa	NIST Webbook
pc	4720.00	kPa	KDB
rinpol	594.00		NIST Webbook
rinpol	582.00		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	616.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	613.00		NIST Webbook
rinpol	626.10		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	619.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	615.00		NIST Webbook
rinpol	594.00		NIST Webbook
rinpol	589.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	599.00		NIST Webbook
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rinpol	603.00		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	606.00		NIST Webbook
rinpol	606.00		NIST Webbook
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rinpol	580.00		NIST Webbook
rinpol	591.00		NIST Webbook
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rinpol	594.00		NIST Webbook
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rinpol	585.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	610.00		NIST Webbook
rinpol	633.00		NIST Webbook
rinpol	608.00		NIST Webbook
rinpol	615.00		NIST Webbook

rinpol	609.00	NIST Webbook
rinpol	609.00	NIST Webbook
rinpol	629.00	NIST Webbook
rinpol	600.00	NIST Webbook
rinpol	605.00	NIST Webbook
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rinpol	604.00	NIST Webbook
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rinpol	593.00	NIST Webbook
rinpol	604.00	NIST Webbook
ripol	880.00	NIST Webbook
ripol	872.00	NIST Webbook
ripol	866.00	NIST Webbook
ripol	866.00	NIST Webbook
ripol	871.00	NIST Webbook
ripol	817.00	NIST Webbook
ripol	853.00	NIST Webbook
ripol	817.00	NIST Webbook
ripol	850.00	NIST Webbook
ripol	875.00	NIST Webbook
ripol	858.00	NIST Webbook
ripol	870.00	NIST Webbook
ripol	872.00	NIST Webbook
ripol	871.00	NIST Webbook
ripol	876.00	NIST Webbook
ripol	876.00	NIST Webbook
ripol	866.00	NIST Webbook
ripol	832.00	NIST Webbook
ripol	871.00	NIST Webbook
ripol	817.00	NIST Webbook
ripol	838.00	NIST Webbook
ripol	843.00	NIST Webbook
ripol	876.00	NIST Webbook
ripol	874.00	NIST Webbook
ripol	872.00	NIST Webbook
ripol	873.00	NIST Webbook
ripol	898.00	NIST Webbook
ripol	837.00	NIST Webbook
ripol	838.00	NIST Webbook
ripol	838.00	NIST Webbook

ripol	838.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	868.00		NIST Webbook
ripol	881.00		NIST Webbook
ripol	888.00		NIST Webbook
ripol	877.00		NIST Webbook
ripol	832.00		NIST Webbook
ripol	858.00		NIST Webbook
ripol	858.00		NIST Webbook
ripol	870.00		NIST Webbook
ripol	863.00		NIST Webbook
ripol	872.00		NIST Webbook
ripol	894.00		NIST Webbook
ripol	864.00		NIST Webbook
ripol	876.00		NIST Webbook
ripol	856.00		NIST Webbook
ripol	872.00		NIST Webbook
ripol	876.00		NIST Webbook
ripol	866.00		NIST Webbook
sl	213.89	J/mol×K	NIST Webbook
tb	336.90 ± 0.60	K	NIST Webbook
tb	336.00 ± 2.00	K	NIST Webbook
tb	337.00 ± 2.00	K	NIST Webbook
tb	337.65 ± 1.50	K	NIST Webbook
tb	336.65 ± 1.00	K	NIST Webbook
tb	337.15 ± 1.50	K	NIST Webbook
tb	338.00 ± 6.00	K	NIST Webbook
tb	336.15 ± 2.00	K	NIST Webbook
tb	337.70	K	NIST Webbook
tb	338.00	K	KDB
tb	337.65 ± 2.00	K	NIST Webbook
tc	528.00 ± 2.00	K	NIST Webbook
tc	527.00	K	KDB
tt	181.90 ± 0.20	K	NIST Webbook
tt	181.90 ± 0.10	K	NIST Webbook
vc	0.247	m3/kmol	KDB
vc	0.247 ± 0.005	m3/kmol	NIST Webbook
zc	0.2660670		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	143.72	J/mol×K	298.15	NIST Webbook
hfust	8.55	kJ/mol	181.90	NIST Webbook
hfust	8.55	kJ/mol	181.90	NIST Webbook
hfust	8.55	kJ/mol	181.90	NIST Webbook
hvapt	32.40	kJ/mol	313.00	NIST Webbook
hvapt	34.40	kJ/mol	294.50	NIST Webbook
hvapt	31.50	kJ/mol	324.00	NIST Webbook
hvapt	32.50	kJ/mol	295.50	NIST Webbook
hvapt	30.90	kJ/mol	353.00	NIST Webbook
pvap	242.70	kPa	367.40	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	162.60	kPa	353.80	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	181.50	kPa	357.50	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	181.70	kPa	357.50	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	186.50	kPa	358.30	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	210.50	kPa	362.40	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives

pvap	211.10	kPa	362.50	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	214.90	kPa	363.10	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	242.10	kPa	367.20	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	161.80	kPa	353.80	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	246.00	kPa	367.90	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	285.30	kPa	373.40	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	286.40	kPa	373.60	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	288.40	kPa	373.90	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	527.60	kPa	398.20	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives

pvap	530.30	kPa	398.40	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	533.80	kPa	398.80	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	587.60	kPa	403.00	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	591.70	kPa	403.20	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	592.30	kPa	403.30	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	667.20	kPa	408.40	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	670.20	kPa	408.60	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	676.70	kPa	409.00	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
rhol	913.00	kg/m3	293.00	KDB

rhol	916.70	kg/m3	295.00	High-pressure vapor-liquid equilibria of the second generation biofuel blends (2-methylfuran + iso-octane) and (2-methyltetrahydrofuran + di-n-butyl ether): Experiments and PCP-SAFT modeling
rhol	910.73	kg/m3	298.15	Excess volumes and partial molar volumes of binary liquid mixtures of furfural or 2-methylfuran with alcohols at 298.15 K
sfust	47.01	J/mol×K	181.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53078e+01
Coeff. B	-3.52676e+03
Coeff. C	-7.07200e+00
Temperature range (K), min.	241.87
Temperature range (K), max.	359.88

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	283.15	928.13
100.00	288.15	922.18
100.00	293.15	916.2

100.00	298.15	910.18
100.00	303.15	904.12
100.00	308.15	898.02
100.00	313.15	891.87
100.00	318.15	885.68
100.00	323.15	879.43
100.00	328.15	873.12
100.00	333.15	866.75
100.00	338.15	860.33
2500.00	283.15	930.56
2500.00	288.15	924.54
2500.00	293.15	918.63
2500.00	298.15	912.71
2500.00	303.15	906.73
2500.00	308.15	900.91
2500.00	313.15	894.72
2500.00	318.15	888.8
2500.00	323.15	882.68
2500.00	328.15	876.29
2500.00	333.15	870.11
2500.00	338.15	863.95
5000.00	283.15	932.75
5000.00	288.15	926.97
5000.00	293.15	921.3
5000.00	298.15	915.3
5000.00	303.15	909.46
5000.00	308.15	903.72
5000.00	313.15	897.62
5000.00	318.15	891.79
5000.00	323.15	885.8
5000.00	328.15	879.75
5000.00	333.15	873.62
5000.00	338.15	867.36
7500.00	283.15	935.07
7500.00	288.15	929.48
7500.00	293.15	923.72
7500.00	298.15	918.0
7500.00	303.15	912.07
7500.00	308.15	906.43
7500.00	313.15	900.57
7500.00	318.15	894.77
7500.00	323.15	888.76
7500.00	328.15	882.71
7500.00	333.15	876.95

7500.00	338.15	870.91
10000.00	283.15	937.27
10000.00	288.15	931.62
10000.00	293.15	926.09
10000.00	298.15	920.32
10000.00	303.15	914.76
10000.00	308.15	909.05
10000.00	313.15	903.14
10000.00	318.15	897.58
10000.00	323.15	891.8
10000.00	328.15	885.92
10000.00	333.15	880.01
10000.00	338.15	874.16
20000.00	283.15	945.74
20000.00	288.15	940.4
20000.00	293.15	934.94
20000.00	298.15	929.72
20000.00	303.15	924.23
20000.00	308.15	918.85
20000.00	313.15	913.34
20000.00	318.15	907.94
20000.00	323.15	902.39
20000.00	328.15	896.99
20000.00	333.15	891.39
20000.00	338.15	886.03
30000.00	283.15	953.37
30000.00	288.15	948.28
30000.00	293.15	943.1
30000.00	298.15	937.91
30000.00	303.15	932.75
30000.00	308.15	927.65
30000.00	313.15	922.45
30000.00	318.15	917.27
30000.00	323.15	911.96
30000.00	328.15	906.92
30000.00	333.15	901.64
30000.00	338.15	896.44
40000.00	283.15	960.5
40000.00	288.15	955.59
40000.00	293.15	950.59
40000.00	298.15	945.67
40000.00	303.15	940.68
40000.00	308.15	935.68
40000.00	313.15	930.83

40000.00	318.15	925.75
40000.00	323.15	920.89
40000.00	328.15	915.88
40000.00	333.15	910.95
40000.00	338.15	905.99
50000.00	283.15	967.21
50000.00	288.15	962.35
50000.00	293.15	957.61
50000.00	298.15	952.89
50000.00	303.15	948.03
50000.00	308.15	943.2
50000.00	313.15	938.5
50000.00	318.15	933.61
50000.00	323.15	929.01
50000.00	328.15	924.13
50000.00	333.15	919.48
50000.00	338.15	914.74
60000.00	283.15	973.54
60000.00	288.15	968.84
60000.00	293.15	964.27
60000.00	298.15	959.58
60000.00	303.15	955.1
60000.00	308.15	950.35
60000.00	313.15	945.71
60000.00	318.15	941.15
60000.00	323.15	936.53
60000.00	328.15	931.92
60000.00	333.15	927.42
60000.00	338.15	922.79
99.00	278.15	934.034
99.00	280.65	931.092
99.00	283.15	928.13
99.00	285.65	925.161
99.00	288.15	922.181
99.00	290.65	919.197
99.00	293.15	916.198
99.00	295.65	913.193
99.00	298.15	910.179
99.00	300.65	907.155
99.00	303.15	904.121
99.00	305.65	901.077
99.00	308.15	898.02
99.00	310.65	894.953
99.00	313.15	891.871

99.00	315.65	888.779
99.00	318.15	885.676
99.00	320.65	882.558
99.00	323.15	879.425
99.00	325.65	876.278
99.00	328.15	873.118
99.00	330.65	869.944
99.00	333.15	866.753
99.00	335.65	863.547
99.00	338.15	860.327

Reference *https://www.doi.org/10.1016/j.tca.2015.08.013*

Sources

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Crippen Method:	https://www.cheric.org/files/research/kdb/mol/mol1036.mol
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Measurement and modeling of infinite dilution activity coefficients of organic compounds in an equimolar ionic liquid mixture of [Bmim]Cl and [Bmim][Tf2N]:	https://www.doi.org/10.1016/j.tca.2015.08.013
NIST Webbook:	https://www.doi.org/10.1016/j.fluid.2019.01.028
Crippen Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C534225&Units=SI
McGowan Method:	https://www.chemeo.com/doc/models/crippen_log10ws
	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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