

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	8.37 ± 0.05	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
ie	8.39 ± 0.01	eV	NIST Webbook
ie	8.39 ± 0.01	eV	NIST Webbook
ie	8.57	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
ie	8.38 ± 0.01	eV	NIST Webbook
ie	8.54	eV	NIST Webbook
ie	8.31 ± 0.09	eV	NIST Webbook
ie	8.37	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	606.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	585.00		NIST Webbook
rinpol	595.00		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	610.00		NIST Webbook
rinpol	633.00		NIST Webbook
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rinpol	629.00	NIST Webbook
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ripol	873.00	NIST Webbook
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ripol	817.00		NIST Webbook
ripol	871.00		NIST Webbook
ripol	832.00		NIST Webbook
ripol	866.00		NIST Webbook
ripol	876.00		NIST Webbook
ripol	880.00		NIST Webbook
ripol	871.00		NIST Webbook
ripol	872.00		NIST Webbook
ripol	858.00		NIST Webbook
ripol	875.00		NIST Webbook
ripol	850.00		NIST Webbook
ripol	870.00		NIST Webbook
ripol	843.00		NIST Webbook
ripol	817.00		NIST Webbook
sl	213.89	J/molxK	NIST Webbook
tb	338.00	K	KDB
tb	338.00 ± 6.00	K	NIST Webbook
tb	337.15 ± 1.50	K	NIST Webbook
tb	336.65 ± 1.00	K	NIST Webbook
tb	337.00 ± 2.00	K	NIST Webbook
tb	336.00 ± 2.00	K	NIST Webbook
tb	336.90 ± 0.60	K	NIST Webbook
tb	337.65 ± 2.00	K	NIST Webbook
tb	337.70	K	NIST Webbook
tb	337.65 ± 1.50	K	NIST Webbook
tb	336.15 ± 2.00	K	NIST Webbook
tc	528.00 ± 2.00	K	NIST Webbook
tc	527.00	K	KDB
tt	181.90 ± 0.10	K	NIST Webbook
tt	181.90 ± 0.20	K	NIST Webbook
vc	0.247 ± 0.005	m ³ /kmol	NIST Webbook
vc	0.247	m ³ /kmol	KDB
zc	0.2660670		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	143.72	J/molxK	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	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
hvapt	34.40	kJ/mol	294.50	NIST Webbook
pvap	286.40	kPa	373.60	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	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	285.30	kPa	373.40	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	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
pvap	246.00	kPa	367.90	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives

rho1	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
rho1	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
rho1	913.00	kg/m3	293.00	KDB
sfust	47.01	J/molxK	181.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Design of Equilibrium Cells for Phase Equilibria and PVT Measurements in Large Ranges of Temperatures and Pressures. I. Vapor Liquid Liquid Equilibria

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Solubility of carbon monoxide in bio-oil compounds:

<https://www.doi.org/10.1016/j.jct.2016.10.030>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C534225&Units=SI>

Isothermal vapor liquid equilibrium for binary mixtures containing furfural and MeO, and modeling of infinite dilution activity coefficients of organic compounds in ionic liquid

<https://www.doi.org/10.1016/j.fluid.2014.10.037>

<https://www.doi.org/10.1016/j.fluid.2019.01.028>

The Yaws Handbook of Vapor Pressure of [Bmim]Cl and [Bmim][Tf2N]: High-pressure vapor-liquid equilibria of the second generation biofuel blends

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<https://www.doi.org/10.1016/j.fluid.2015.05.002>

Excess volumes and partial molar volumes of binary liquid mixtures of furfural with n-butyl alcohol and 2-methyltetrahydrofuran + di-n-butyl ether. Experiments and PC-SAFT

<http://link.springer.com/article/10.1007/BF02311772>

<https://www.doi.org/10.1016/j.jct.2019.02.027>

<https://www.doi.org/10.1016/j.tca.2015.08.013>

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
rho:	Liquid Density
rinp:	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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