Furan, 2,5-dimethyl-

Other names:	2,5-Dimethylfuran
	2,5-Dimethylfurane
	2,5-dimethyloxole
Inchi:	InChI=1S/C6H8O/c1-5-3-4-6(2)7-5/h3-4H,1-2H3
InchiKey:	GSNUFIFRDBKVIE-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	Cc1ccc(C)o1
Mol. weight [g/mol]:	96.13
CAS:	625-86-5

Physical Properties

Property code	Value	Unit	Source
affp	865.90	kJ/mol	NIST Webbook
basg	835.20	kJ/mol	NIST Webbook
hvap	31.80 ± 0.30	kJ/mol	NIST Webbook
ie	8.03	eV	NIST Webbook
ie	8.25 ± 0.10	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-6.16		Crippen Method
logp	1.896		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	701.00		NIST Webbook
rinpol	685.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	684.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	728.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	693.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	711.00		NIST Webbook
rinpol	723.00		NIST Webbook
rinpol	707.00		NIST Webbook
rinpol	700.00		NIST Webbook
rinpol	715.00		NIST Webbook
rinpol	700.00		NIST Webbook

rinpol	712.00	NIST Webbook
rinpol	727.00	NIST Webbook
rinpol	728.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	703.00	NIST Webbook
rinpol	708.00	NIST Webbook
rinpol	694.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	700.00	NIST Webbook
rinpol	707.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	689.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	712.00	NIST Webbook
rinpol	703.00	NIST Webbook
rinpol	707.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	706.00	NIST Webbook
rinpol	723.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	696.00	NIST Webbook
rinpol	718.00	NIST Webbook
rinpol	701.00	NIST Webbook
rinpol	667.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	697.00	NIST Webbook
rinpol	695.00	NIST Webbook
rinpol	696.00	NIST Webbook
ripol	943.00	NIST Webbook
ripol	938.00	NIST Webbook
ripol	890.00	NIST Webbook
ripol	950.00	NIST Webbook
ripol	925.00	NIST Webbook
ripol	930.00	NIST Webbook
ripol	958.00	NIST Webbook
ripol	958.00	NIST Webbook
ripol	952.00	NIST Webbook
ripol	958.00	NIST Webbook

ripol	946.00		NIST Webbook
ripol	925.00		NIST Webbook
ripol	934.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	931.00		NIST Webbook
ripol	933.00		NIST Webbook
ripol	933.00		NIST Webbook
ripol	933.00		NIST Webbook
ripol	934.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	909.00		NIST Webbook
ripol	943.00		NIST Webbook
ripol	972.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	952.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	949.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	892.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	938.00		NIST Webbook
ripol	939.00		NIST Webbook
ripol	939.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	931.00		NIST Webbook
ripol	943.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	934.00		NIST Webbook
ripol	939.00		NIST Webbook
ripol	953.00		NIST Webbook
tb	366.83	K	Vapor Liquid Equilibrium, Densities, and Interfacial Tensions of the System Hexane + 2,5-Dimethylfuran

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hvapt	32.30 ± 0.30	kJ/mol	289.50	NIST Webbook
pvap	46.74	kPa	343.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
pvap	66.08	kPa	353.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
pvap	13.94	kPa	313.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
pvap	21.54	kPa	323.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
pvap	32.20	kPa	333.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures

pvap	91.23	kPa	363.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
pvap	123.28	kPa	373.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
pvap	163.43	kPa	383.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
pvap	212.88	kPa	393.15	Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures
rfi	1.44012		298.15	Isobaric vapor liquid equilibrium and isothermal surface tensions of 2,2 -oxybis[propane] + 2,5-Dimethylfuran
rfi	1.44012		298.15	Isobaric Vapor Liquid Equilibrium and Isothermal Interfacial Tensions for the System Ethanol + 2,5-Dimethylfuran

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48188e+01
Coeff. B	-3.30555e+03
Coeff. C	-4.29400e+01
Temperature range (K), min.	270.42
Temperature range (K), max.	390.63

Datasets

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	283.15	912.25
100.00	288.15	906.99
100.00	293.15	901.64
100.00	298.15	896.29
100.00	303.15	890.9
100.00	308.15	885.45
100.00	313.15	879.93
100.00	318.15	874.44
100.00	323.15	868.85
100.00	328.15	863.25
100.00	333.15	857.58
100.00	338.15	851.85
2500.00	283.15	914.37
2500.00	288.15	909.13
2500.00	293.15	903.82
2500.00	298.15	898.6
2500.00	303.15	893.25
2500.00	308.15	887.9
2500.00	313.15	882.45
2500.00	318.15	877.03

2500.00	323.15	871.55
2500.00	328.15	866.05
2500.00	333.15	860.47
2500.00	338.15	854.88
5000.00	283.15	916.47
5000.00	288.15	911.29
5000.00	293.15	906.07
5000.00	298.15	900.94
5000.00	303.15	895.65
5000.00	308.15	890.36
5000.00	313.15	885.02
5000.00	318.15	879.68
5000.00	323.15	874.3
5000.00	328.15	868.91
5000.00	333.15	863.42
5000.00	338.15	857.96
7500.00	283.15	918.52
7500.00	288.15	913.42
7500.00	293.15	908.26
7500.00	298.15	903.16
7500.00	303.15	897.97
7500.00	308.15	892.78
7500.00	313.15	887.51
7500.00	318.15	882.27
7500.00	323.15	876.94
7500.00	328.15	871.68
7500.00	333.15	866.28
7500.00	338.15	860.93
10000.00	283.15	920.53
10000.00	288.15	915.49
10000.00	293.15	910.4
10000.00	298.15	905.39
10000.00	303.15	900.25
10000.00	308.15	895.14
10000.00	313.15	889.95
10000.00	318.15	884.79
10000.00	323.15	879.54
10000.00	328.15	874.38
10000.00	333.15	869.07
10000.00	338.15	863.81
20000.00	283.15	928.2
20000.00	288.15	923.34
20000.00	293.15	918.5
20000.00	298.15	913.73

20000.00	303.15	908.83
20000.00	308.15	903.98
20000.00	313.15	899.05
20000.00	318.15	894.18
20000.00	323.15	889.25
20000.00	328.15	884.36
20000.00	333.15	879.4
20000.00	338.15	874.45
30000.00	283.15	935.24
30000.00	288.15	930.62
30000.00	293.15	925.97
30000.00	298.15	921.4
30000.00	303.15	916.74
30000.00	308.15	912.1
30000.00	313.15	907.41
30000.00	318.15	902.74
30000.00	323.15	898.07
30000.00	328.15	893.38
30000.00	333.15	888.7
30000.00	338.15	884.02
40000.00	283.15	941.89
40000.00	288.15	937.41
40000.00	293.15	932.94
40000.00	298.15	928.44
40000.00	303.15	924.06
40000.00	308.15	919.56
40000.00	313.15	915.12
40000.00	318.15	910.6
40000.00	323.15	906.13
40000.00	328.15	901.61
40000.00	333.15	897.22
40000.00	338.15	892.61
50000.00	283.15	948.12
50000.00	288.15	943.72
50000.00	293.15	939.57
50000.00	298.15	935.19
50000.00	303.15	930.89
50000.00	308.15	926.54
50000.00	313.15	922.3
50000.00	318.15	917.91
50000.00	323.15	913.67
50000.00	328.15	909.29
50000.00	333.15	905.17
50000.00	338.15	900.74

60000.00	283.15	953.98
60000.00	288.15	949.78
60000.00	293.15	945.6
60000.00	298.15	941.44
60000.00	303.15	937.27
60000.00	308.15	933.08
60000.00	313.15	928.9
60000.00	318.15	924.74
60000.00	323.15	920.58
60000.00	328.15	916.43
60000.00	333.15	912.4
60000.00	338.15	908.17
99.00	278.15	917.53
99.00	280.65	914.899
99.00	283.15	912.247
99.00	285.65	909.614
99.00	288.15	906.988
99.00	290.65	904.299
99.00	293.15	901.636
99.00	295.65	898.951
99.00	298.15	896.285
99.00	300.65	893.569
99.00	303.15	890.898
99.00	305.65	888.151
99.00	308.15	885.447
99.00	310.65	882.693
99.00	313.15	879.927
99.00	315.65	877.195
99.00	318.15	874.437
99.00	320.65	871.651
99.00	323.15	868.85
99.00	325.65	866.06
99.00	328.15	863.248
99.00	330.65	860.418
99.00	333.15	857.577
99.00	335.65	854.721
99.00	338.15	851.85

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

Sources

Isobaric vapor liquid equilibrium and isothermal surface tensions of 2,2 -oxybis[propane] + 2,5-Dimethylfuran:	https://www.doi.org/10.1016/j.fluid.2013.02.005
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C625865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Isobaric Vapor Liquid Equilibrium and Isothermal Interfacial Tensions for the System Ethanol + 2,5-Dimethylfuran:	https://www.doi.org/10.1021/je400683g
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermophysical study of the furan family:	https://www.doi.org/10.1016/j.tca.2015.08.013
Vapor Liquid Equilibrium, Densities, and Interfacial Tensions of the System Hexane + 2,5-Dimethylfuran :	https://www.doi.org/10.1021/je300631s
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Phase equilibrium properties of binary mixtures containing 2,5-dimethylfuran and furfuryl alcohol or methyl isobutyl ketone at several temperatures:	https://www.doi.org/10.1016/j.jct.2013.10.039
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.fluid.2019.01.028

Legend

affp:	Proton affinity
basg:	Gas basicity
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
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature