Furan

Other names:	1,4-Epoxy-1,3-butadiene
	DIVINYLENE OXIDE
	Furane
	Furfuran
	Furfurane
	NCI-C56202
	OXACYCLOPENTADIENE
	OXOLE
	Rcra waste number U124
	Tetrole
	UN 2389
Inchi:	InChI=1S/C4H4O/c1-2-4-5-3-1/h1-4H
InchiKey:	YLQBMQCUIZJEEH-UHFFFAOYSA-N
Formula:	C4H4O
SMILES:	c1ccoc1
Mol. weight [g/mol]:	68.07
CAS:	110-00-9

Physical Properties

Property code	Value	Unit	Source
af	0.2090		KDB
affp	803.40	kJ/mol	NIST Webbook
affp	812.00 ± 8.00	kJ/mol	NIST Webbook
affp	813.00 ± 8.00	kJ/mol	NIST Webbook
basg	782.00 ± 8.00	kJ/mol	NIST Webbook
basg	781.00 ± 8.00	kJ/mol	NIST Webbook
basg	770.90	kJ/mol	NIST Webbook
dm	0.70	debye	KDB
gf	0.88	kJ/mol	KDB
hf	-34.70	kJ/mol	NIST Webbook
hf	-27.70	kJ/mol	NIST Webbook
hf	-29.80	kJ/mol	NIST Webbook
hf	-34.70	kJ/mol	KDB
hvap	27.71	kJ/mol	NIST Webbook
hvap	28.20	kJ/mol	NIST Webbook
hvap	27.60	kJ/mol	NIST Webbook
ie	8.89 ± 0.05	eV	NIST Webbook

ie	8.88	eV	NIST Webbook
ie	8.89	eV	NIST Webbook
ie	8.89	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.88 ± 0.01	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
ie	8.98 ± 0.03	eV	NIST Webbook
ie	8.83	eV	NIST Webbook
ie	8.87	eV	NIST Webbook
ie	8.89 ± 0.01	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
ie	8.88 ± 0.05	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.89	eV	NIST Webbook
ie	8.85 ± 0.05	eV	NIST Webbook
ie	8.99 ± 0.05	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
ie	8.88	eV	NIST Webbook
ie	8.91 ± 0.01	eV	NIST Webbook
ie	8.87 ± 0.03	eV	NIST Webbook
ie	8.83	eV	NIST Webbook
log10ws	-0.82		Aqueous Solubility Prediction Method
log10ws	-0.82		Estimated Solubility Method
logp	1.280		Crippen Method
mcvol	53.630	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=1)		KDB
nfpas	%!d(float64=1)		KDB
pc	5320.00 ± 117.20	kPa	NIST Webbook
pc	5500.00	kPa	KDB
rinpol	495.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	483.00		NIST Webbook
rinpol	498.00		NIST Webbook
rinpol	485.00		NIST Webbook
rinpol	500.00		NIST Webbook
rinpol	131.10		NIST Webbook
rinpol	492.00		NIST Webbook
rinpol	500.00		NIST Webbook

rinpol	500.00		NIST Webbook
rinpol	492.00		NIST Webbook
rinpol	495.00		NIST Webbook
ripol	779.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	831.00		NIST Webbook
ripol	798.00		NIST Webbook
ripol	786.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	786.00		NIST Webbook
ripol	760.00		NIST Webbook
ripol	831.00		NIST Webbook
ripol	800.00		NIST Webbook
ripol	813.00		NIST Webbook
ripol	827.00		NIST Webbook
ripol	801.00		NIST Webbook
ripol	802.00		NIST Webbook
ripol	802.00		NIST Webbook
ripol	786.00		NIST Webbook
ripol	797.00		NIST Webbook
ripol	802.00		NIST Webbook
ripol	797.00		NIST Webbook
ripol	790.00		NIST Webbook
ripol	798.00		NIST Webbook
ripol	802.00		NIST Webbook
tb	304.15 ± 1.00	K	NIST Webbook
tb	304.60	K	KDB
tb	304.60	K	NIST Webbook
tb	304.50	K	NIST Webbook
tb	307.15 ± 3.00	K	NIST Webbook
tb	304.51 ± 0.05	K	NIST Webbook
tb	305.15 ± 5.00	K	NIST Webbook
tb	305.15 ± 0.70	K	NIST Webbook
tb	305.15 ± 1.00	K	NIST Webbook
tb	304.42 ± 0.25	K	NIST Webbook
tb	304.75 ± 0.30	K	NIST Webbook
tb	304.47 ± 0.20	K	NIST Webbook
tb	305.00 ± 2.00	K	NIST Webbook
tb	304.48 ± 0.08	K	NIST Webbook
tc	487.00 ± 2.00	K	NIST Webbook
tc	490.20 ± 0.30	K	NIST Webbook
tc	490.20	K	NIST Webbook
tc	490.20	K	KDB
tf	187.56 ± 0.05	K	NIST Webbook

tf	187.15 ± 1.00	K	NIST Webbook
tf	187.50	K	KDB
tf	187.75	K	Aqueous Solubility Prediction Method
tf	187.55 ± 0.30	K	NIST Webbook
tf	187.44 ± 0.20	K	NIST Webbook
tf	187.47 ± 0.20	K	NIST Webbook
tt	187.55 ± 0.02	K	NIST Webbook
tt	187.54 ± 0.05	K	NIST Webbook
vc	0.219 ± 0.005	m3/kmol	NIST Webbook
vc	0.218	m3/kmol	KDB
zc	0.2941770		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.58	J/mol×K	449.20	NIST Webbook
cpg	90.00	J/mol×K	402.20	NIST Webbook
cpg	80.12	J/mol×K	358.20	NIST Webbook
cpg	70.29	J/mol×K	317.25	NIST Webbook
cpg	106.48	J/mol×K	487.20	NIST Webbook
hfust	3.80	kJ/mol	187.60	NIST Webbook
hfust	3.80	kJ/mol	187.60	NIST Webbook
hfust	2.05	kJ/mol	150.00	NIST Webbook
hvapt	30.20	kJ/mol	297.00	NIST Webbook
hvapt	27.70	kJ/mol	304.36	NIST Webbook
hvapt	28.60	kJ/mol	304.50	NIST Webbook
hvapt	27.20	kJ/mol	304.20	NIST Webbook
hvapt	27.10	kJ/mol	304.50	NIST Webbook
hvapt	27.45	kJ/mol	298.15	NIST Webbook
hvapt	27.09	kJ/mol	304.50	KDB
pvap	1513.30	kPa	407.90	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
pvap	735.60	kPa	373.10	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives

pvap	455.10	kPa	353.40	Isothermal vapor liquid equilibrium for binary mixtures containing furfural and its derivatives
rfi	1.42100		293.15	Solubility of hydrogen in bio-oil compounds
rhol	938.00	kg/m3	293.00	KDB
sfust	20.29	J/mol×K	187.60	NIST Webbook
sfust	13.64	J/mol×K	150.00	NIST Webbook
svapt	92.07	J/mol×K	298.15	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	305.20	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43852e+01
Coeff. B	-2.63288e+03
Coeff. C	-3.51270e+01
Temperature range (K), min.	221.89
Temperature range (K), max.	490.15

Datasets

Refractive index (Na D-line)

Pressure, kPa - Liquid	Temperature, K - Liquid	Refractive index (Na D-line) - Liquid
101.23	293.15	1.4218

Reference *https://www.doi.org/10.1021/acs.jced.6b00424*

Mass density, kg/m3

Pressure, kPa - Liquid	Temperature, K - Liquid	Mass density, kg/m3 - Liquid
100.00	283.15	952.36
100.00	288.15	945.58
100.00	293.15	938.74
100.00	298.15	931.84
100.00	303.15	924.86
2500.00	283.15	954.38
2500.00	288.15	947.81
2500.00	293.15	940.99
2500.00	298.15	934.31
2500.00	303.15	927.4
2500.00	308.15	920.6
2500.00	313.15	913.48
2500.00	318.15	906.59
2500.00	323.15	899.25
2500.00	328.15	892.18
2500.00	333.15	884.69
2500.00	338.15	877.34
5000.00	283.15	956.94
5000.00	288.15	950.42
5000.00	293.15	943.7
5000.00	298.15	937.14
5000.00	303.15	930.33
5000.00	308.15	923.71
5000.00	313.15	916.68
5000.00	318.15	909.88
5000.00	323.15	902.71
5000.00	328.15	895.9
5000.00	333.15	888.51
5000.00	338.15	881.44
7500.00	283.15	959.39
7500.00	288.15	953.03
7500.00	293.15	946.38

7500.00	298.15	939.92
7500.00	303.15	933.21
7500.00	308.15	926.73
7500.00	313.15	919.8
7500.00	318.15	913.18
7500.00	323.15	906.1
7500.00	328.15	899.49
7500.00	333.15	892.17
7500.00	338.15	885.37
10000.00	283.15	961.81
10000.00	288.15	955.59
10000.00	293.15	948.97
10000.00	298.15	942.68
10000.00	303.15	936.0
10000.00	308.15	929.66
10000.00	313.15	922.81
10000.00	318.15	916.44
10000.00	323.15	909.42
10000.00	328.15	902.97
10000.00	333.15	895.74
10000.00	338.15	889.16
20000.00	283.15	970.97
20000.00	288.15	965.03
20000.00	293.15	958.75
20000.00	298.15	952.79
20000.00	303.15	946.46
20000.00	308.15	940.5
20000.00	313.15	934.04
20000.00	318.15	928.06
20000.00	323.15	921.53
20000.00	328.15	915.52
20000.00	333.15	908.84
20000.00	338.15	902.71
30000.00	283.15	979.35
30000.00	288.15	973.69
30000.00	293.15	967.71
30000.00	298.15	961.99
30000.00	303.15	956.04
30000.00	308.15	950.3
30000.00	313.15	944.27
30000.00	318.15	938.56
30000.00	323.15	932.47
30000.00	328.15	926.72
30000.00	333.15	920.52

30000.00	338.15	914.72
40000.00	283.15	987.2
40000.00	288.15	981.69
40000.00	293.15	976.04
40000.00	298.15	970.53
40000.00	303.15	964.82
40000.00	308.15	959.34
40000.00	313.15	953.57
40000.00	318.15	948.09
40000.00	323.15	942.39
40000.00	328.15	936.8
40000.00	333.15	931.04
40000.00	338.15	925.5
50000.00	283.15	994.5
50000.00	288.15	989.18
50000.00	293.15	983.77
50000.00	298.15	978.42
50000.00	303.15	972.99
50000.00	308.15	967.69
50000.00	313.15	962.21
50000.00	318.15	956.88
50000.00	323.15	951.44
50000.00	328.15	946.08
50000.00	333.15	940.62
50000.00	338.15	935.32
60000.00	283.15	1001.42
60000.00	288.15	996.21
60000.00	293.15	990.98
60000.00	298.15	985.81
60000.00	303.15	980.62
60000.00	308.15	975.44
60000.00	313.15	970.23
60000.00	318.15	965.06
60000.00	323.15	959.86
60000.00	328.15	954.71
60000.00	333.15	949.48
60000.00	338.15	944.34
99.00	278.15	959.086
99.00	280.65	955.729
99.00	283.15	952.358
99.00	285.65	948.976
99.00	288.15	945.579
99.00	290.65	942.167
99.00	293.15	938.739

99.00	295.65	935.294
99.00	298.15	931.835
99.00	300.65	928.357
99.00	303.15	924.861

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

Sources

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Isothermal vapor-liquid equilibrium for binary mixtures containing furfural and its derivatives:	https://www.doi.org/10.1016/j.fluid.2014.10.037
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NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110009&Units=SI
Thermophysical study of the furan family:	https://www.doi.org/10.1016/j.tca.2015.08.013
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Solubility of hydrogen in bio-oil compounds:	https://www.doi.org/10.1016/j.jct.2016.07.010
Vapour-liquid equilibrium (VLE) for the systems furan + n-hexane and furan + toluene. Measurements, data treatment and modeling using molecular models:	https://www.doi.org/10.1016/j.fluid.2012.08.005
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Solubility of carbon monoxide in bio-oil compounds:	https://www.doi.org/10.1016/j.jct.2016.10.030
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility