Furan, tetrahydro-2-methyl-

Other names:	.alpha.-methyltetramethylene oxide
	2-Methylfuranidine
	2-Methyloxolane
	2-Methyltetrahydrofuran
	2-Methyltetrahydrofurane
	Furan, 2-methyl-tetrahydro-
	Methyltetrahydrofuran
	Tetrahydro-2-methylfuran
	Tetrahydrofuran, 2-methyl-
	Tetrahydrosylvan
Inchi:	InChI=1S/C5H10O/c1-5-3-2-4-6-5/h5H,2-4H2,1H3
InchiKey:	JWUJQDFVADABEY-UHFFFAOYSA-N
Formula:	C5H10O
SMILES:	CC1CCCO1
Mol. weight [g/mol]:	86.13
CAS:	96-47-9

Physical Properties

Property code	Value	Unit	Source
affp	840.80	kJ/mol	NIST Webbook
basg	811.60	kJ/mol	NIST Webbook
gf	-58.35	kJ/mol	Joback Method
hf	-218.05	kJ/mol	Joback Method
hfus	10.62	kJ/mol	Joback Method
hvap	34.00	kJ/mol	NIST Webbook
hvap	33.70	kJ/mol	NIST Webbook
ie	9.22 ± 0.05	eV	NIST Webbook
log10ws	0.11		Aqueous Solubility Prediction Method
log10ws	0.11		Estimated Solubility Method
logp	1.185		Crippen Method
mcvol	76.320	ml/mol	McGowan Method
pc	3757.63 ± 68.94	kPa	NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	682.00		NIST Webbook
rinpol	661.00		NIST Webbook

rinpol	678.00		NIST Webbook
rinpol	669.00		NIST Webbook
rinpol	663.00		NIST Webbook
rinpol	674.00		NIST Webbook
rinpol	664.00		NIST Webbook
rinpol	663.00		NIST Webbook
ripol	876.00		NIST Webbook
ripol	925.00		NIST Webbook
ripol	951.00		NIST Webbook
ripol	925.00		NIST Webbook
ripol	935.00		NIST Webbook
ripol	876.00		NIST Webbook
tb	338.15 ± 2.00	K	NIST Webbook
tb	353.15 ± 1.00	K	NIST Webbook
tb	359.65 ± 1.00	K	NIST Webbook
tb	353.10 ± 0.30	K	NIST Webbook
tb	353.20	K	NIST Webbook
tb	352.65 ± 2.00	K	NIST Webbook
tc	537.00 ± 2.00	K	NIST Webbook
tf	137.05 ± 0.40	K	NIST Webbook
vc	0.267 ± 0.005	m3/kmol	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.02	J/mol×K	421.80	Joback Method
cpg	129.20	J/mol×K	356.03	Joback Method
cpg	141.40	J/mol×K	388.92	Joback Method
cpg	194.00	J/mol×K	553.34	Joback Method
cpg	184.54	J/mol×K	520.46	Joback Method
cpg	174.57	J/mol×K	487.57	Joback Method
cpg	164.07	J/mol×K	454.69	Joback Method
cpl	160.20	J/mol×K	308.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K

cpl	153.50	J/mol×K	288.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
cpl	155.30	J/mol×K	293.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
cpl	162.10	J/mol×K	313.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
cpl	158.70	J/mol×K	303.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K

cpl	164.20	J/mol×K	318.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
cpl	166.20	J/mol×K	323.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
cpl	155.30	J/mol×K	293.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Poly(ethylene glycols) + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
cpl	158.60	J/mol×K	303.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Poly(ethylene glycols) + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
cpl	162.10	J/mol×K	313.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Poly(ethylene glycols) + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K

cpl	156.90	J/mol×K	298.15	Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Dimethyl Sulfoxide + Tetrahydropyran and + 2-Methyltetrahydrofuran at (293.15, 303.15, and 313.15) K
dvisc	0.0005618	Pa×s	283.15	Excess Enthalpy, Density, Speed of Sound, and Viscosity for 2-Methyltetrahydrofuran + 1-Butanol at (283.15, 298.15, and, 313.15) K
dvisc	0.0004776	Pa×s	298.15	Excess Enthalpy, Density, Speed of Sound, and Viscosity for 2-Methyltetrahydrofuran + 1-Butanol at (283.15, 298.15, and, 313.15) K
dvisc	0.0004088	Pa×s	313.15	Excess Enthalpy, Density, Speed of Sound, and Viscosity for 2-Methyltetrahydrofuran + 1-Butanol at (283.15, 298.15, and, 313.15) K
kvisc	0.0000006	m2/s	298.15	Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methyltetrahydrofuran
kvisc	0.0000005	m2/s	313.15	Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with 2-Methyltetrahydrofuran

pvap	18.28	kPa	306.05	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	11.65	kPa	295.94	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	9.26	kPa	291.17	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	21.69	kPa	310.11	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	7.83	kPa	287.83	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	6.57	kPa	284.34	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	13.37	kPa	298.94	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	5.60	kPa	281.41	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	4.93	kPa	279.01	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	4.93	kPa	279.00	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	15.76	kPa	302.62	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	7.85	kPa	287.84	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	5.63	kPa	281.44	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
rfi	1.40287		298.15	Thermophysical properties of the binary mixtures of 2-methyl-tetrahydrofuran with benzene and halobenzenes
rfi	1.40299		298.00	Quaternary and ternary LLE measurements for solvent (2-methyltetrahydrofuran and cyclopentyl methyl ether) + furfural + acetic acid + water between 298 and 343 K
rfi	1.40280		298.15	Ternary and binary LLE measurements for solvent (2-methyltetrahydrofuran and cyclopentyl methyl ether) + furfural + water between 298 and 343 K

rhol	848.10	kg/m3	298.15	Excess molar enthalpies of the ternary mixtures (1-hexene + tetrahydrofuran or 2-methyltetrahydrofuran + methyl tert-butyl ether) at the temperature 298.15K.
rhol	848.10	kg/m3	298.15	Excess molar enthalpies of the ternary mixtures: (tetrahydrofuran or 2-methyltetrahydrofuran + methyl tert-butyl ether + n-octane) at the temperature 298.15 K
rhol	848.10	kg/m3	298.15	Excess molar enthalpies of the ternary mixtures: {tetrahydrofuran or 2-methyltetrahydrofuran + methyl tert-butyl ether + n-dodecane} at the temperature 298.15 K
rhol	855.00	kg/m3	293.15	Isothermal Vapor-Liquid Equilibrium Data for the Binary Systems Consisting of 1,1,2,3,3,3-Hexafluoro-1-propene and Either Methylcyclohexane, Cyclohexane, n-Hexane, 2-Methyltetrahydrofuran, or 2,2,3,3,4,4,4-Heptafluoro-1-butanol
rhol	849.40	kg/m3	298.15	Study of the Surface Tension of Chlorocyclohexane or Bromocyclohexane with Some Cyclic Ethers
rhol	849.20	kg/m3	298.15	Thermodynamic study of 2-methyl-tetrahydrofuran with isomeric chlorobutanes

rhol	851.60	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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47976e+01
Coeff. B	-3.18218e+03
Coeff. C	-3.93870e+01
Temperature range (K), min.	258.70
Temperature range (K), max.	374.84

Sources

Viscosities of Binary Mixtures of Isomeric Butanols or Isomeric Chlorobutanes with	https://www.doi.org/10.1021/je030167i
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
2-Methyltetrahydrofuran:	
Ternary and binary LLE measurements for solvent (2-methyltetrahydrofuran and cyclopentyl methyl ether) + furfural + water between 298 and 343 K:	https://www.doi.org/10.1016/j.jct.2017.02.016
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Excess molar enthalpies of the ternary mixtures: {tetrahydrofuran or 2-methyltetrahydrofuran + methyl	https://www.doi.org/10.1016/j.jct.2004.12.005
Excess molar enthalpies of the ternary mixtures (1-hexene + tetrahydrofuran	https://www.doi.org/10.1016/j.jct.2006.03.020
High-pressure vapor-liquid equilibria of the second generation biofuel blends	https://www.doi.org/10.1016/j.fluid.2015.05.002
Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Thermophysical properties of the binary mixtures of	https://www.doi.org/10.1016/j.tca.2005.08.034
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Isothermal Vapor-Liquid Equilibrium Data for the Binary Systems Consisting	https://www.doi.org/10.1021/acs.jced.9b00441
Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of	https://www.doi.org/10.1021/je600557n
Excess Enthalpy, Density, Speed of	https://www.doi.org/10.1021/je060017i
Ternary and binary LLE measurements for solvent (2-methyltetrahydrofuran and cyclopentyl methyl ether) + furfural + water between 298 and 343 K:	https://www.doi.org/10.1016/j.jct.2005.07.017

Liquid-liquid equilibrium of 2-methyltetrahydrofuran/water over wide temperature range: Measurements and correlation	https://www.doi.org/10.1016/j.fluid.2016.11.004
Excess molar enthalpies of the ternary mixtures {methyl tert-butyl ether or 2-methyltetrahydrofuran + cyclohexane or 1-chlorobutane} at the temperature 298.15 K.	https://www.doi.org/10.1016/j.jct.2004.09.003
Study of the Surface Tension of 2-Methyltetrahydrofuran + Cyclohexane, + Chlorocyclohexane, or + Methylcyclohexane at Various Temperatures	https://www.doi.org/10.1021/je0500577
McGowan's Molecular Volumes	http://link.springer.com/article/10.1007/BF02311772
Liquid-Liquid Equilibria with Some Cyclic Ethers.	
Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols.	https://www.doi.org/10.1021/acs.jced.6b00576
Solubility Measurement and Thermodynamic Modeling of Lidocaine in 12 Pure Solvents at Temperatures Ranging from 278.15 K to 318.15 K:	https://www.doi.org/10.1021/acs.jced.7b01011
NIST Webbook, Ethanol, 2-chloro-N-(2,3-dimethylphenyl)-	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96479&Units=SI
Thermodynamic study of 2-methyl-tetrahydrofuran with isomeric chlorobutanes:	https://www.doi.org/10.1016/j.tca.2004.11.034
Molar Heat Capacities, Densities, Viscosities, and Refractive Indices of Poly(ethylene glycols)	https://www.doi.org/10.1021/je7003066
Quaternary and ternary LLE measurements for solvent 2-methyltetrahydrofuran at (293.15, 303.15, and 313.15) K.	https://www.doi.org/10.1016/j.jct.2017.12.015
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
2-methyltetrahydrofuran and cyclopentyl methyl ether) + furfural + acetic acid + water between 298 and 343 K:	

Legend

affp:	Proton affinity
basg:	Gas basicity
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
kvisc:	Kinematic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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