

Ethanone, 1-(2-furanyl)-

Other names:	(2-Furanyl)-1-ethanone 1-(2-Furanyl)-ethanone (2-acetylfuran) 1-(2-Furanyl)ethanone 1-(2-furanyl)ethanone (acetylfuran) 2-Acetylfurane 2-acetylfuran 2-furyl methyl ketone Acetylfuran Furan, 2-acetyl- Ketone, 2-furyl methyl Methyl 2-furyl ketone furyl methyl ketone
Inchi:	InChI=1S/C6H6O2/c1-5(7)6-3-2-4-8-6/h2-4H,1H3
InchiKey:	IEMMBWWQXVXBEU-UHFFFAOYSA-N
Formula:	C6H6O2
SMILES:	CC(=O)c1ccco1
Mol. weight [g/mol]:	110.11
CAS:	1192-62-7

Physical Properties

Property code	Value	Unit	Source
hfus	15.51	kJ/mol	Enthalpies of combustion and formation of 2-acetylpyrrole, 2-acetylfuran and 2-acetylthiophene
hvap	53.00 ± 0.60	kJ/mol	NIST Webbook
ie	9.02	eV	NIST Webbook
ie	9.27 ± 0.05	eV	NIST Webbook
log10ws	-5.87		Crippen Method
logp	1.482		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
rinpol	923.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	895.00		NIST Webbook

rinpol	896.00	NIST Webbook
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ripol	1510.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1534.00		NIST Webbook
tb	446.00	K	NIST Webbook
tf	306.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	15.50	kJ/mol	301.60	NIST Webbook
pvap	8.03	kPa	370.55	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	2.01	kPa	342.65	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

pvap	3.06	kPa	349.75	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	3.62	kPa	353.35	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	4.02	kPa	355.05	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	5.18	kPa	360.65	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	6.02	kPa	363.95	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

pvap	7.03	kPa	367.65	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	1.54	kPa	337.95	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	9.03	kPa	373.55	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	10.04	kPa	376.35	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	15.04	kPa	386.55	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

pvap	20.07	kPa	394.15	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	29.89	kPa	405.55	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	39.93	kPa	414.25	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	3.60	kPa	353.10	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa
pvap	5.18	kPa	360.86	Vapor Pressure and Isobaric Vapor-Liquid Equilibrium for Binary Systems of Furfural, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
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tbrp	340.20	K	1.30	NIST Webbook
tbrp	340.00	K	1.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Enthalpies of combustion and formation of 2-acetylpyrrole, 2-acetylfuran and 2-acetylthiophene:	https://www.doi.org/10.1016/j.tca.2009.04.012
Vapor-Liquid Equilibrium for Binary Systems: Methanol, 2-Acetylfuran, and 5-Methylfurfural at 3.60 and 5.18 kPa:	https://www.doi.org/10.1021/acs.jced.7b00574
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192627&Units=SI

Legend

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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