Ethanone, 1-cyclopropyl-

Other names:	1-Cyclopropylethanone
	1-cyclopropyl ethanone
	1-cyclopropyl-1-ethanone
	Ketone, cyclopropyl methyl
	NSC 1940
	acetylcyclopropane
	cyclopropane, acetyl-
	cyclopropyl methyl ketone
	methyl cyclopropyl ketone
Inchi:	InChI=1S/C5H8O/c1-4(6)5-2-3-5/h5H,2-3H2,1H3
InchiKey:	HVCFCNAITDHQFX-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	CC(=O)C1CC1
Mol. weight [g/mol]:	84.12
CAS:	765-43-5

Physical Properties

Property code	Value	Unit	Source
affp	854.90	kJ/mol	NIST Webbook
basg	823.00	kJ/mol	NIST Webbook
chl	-2916.00	kJ/mol	NIST Webbook
chl	-2956.20 ± 1.00	kJ/mol	NIST Webbook
gf	-76.95	kJ/mol	Joback Method
hf	-115.30 ± 1.20	kJ/mol	NIST Webbook
hfl	-154.70 ± 1.20	kJ/mol	NIST Webbook
hfus	8.44	kJ/mol	Joback Method
hvap	39.47	kJ/mol	NIST Webbook
hvap	39.41 ± 0.09	kJ/mol	NIST Webbook
hvap	39.40 ± 0.10	kJ/mol	NIST Webbook
ie	9.50	eV	NIST Webbook
ie	9.46	eV	NIST Webbook
log10ws	-0.85		Crippen Method
logp	0.985		Crippen Method
mcvol	72.020	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
rinpol	704.00		NIST Webbook
rinpol	704.00		NIST Webbook

rinpol	730.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	706.00		NIST Webbook
tb	384.40	K	NIST Webbook
tb	387.20	K	NIST Webbook
tb	387.00	K	NIST Webbook
tb	384.00 ± 3.00	K	NIST Webbook
tb	384.35 ± 0.50	K	NIST Webbook
tc	568.80	K	Joback Method
tf	204.85 ± 0.30	K	NIST Webbook
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.98	J/mol×K	374.41	Joback Method
cpg	135.15	J/mol×K	406.81	Joback Method
cpg	144.73	J/mol×K	439.21	Joback Method
cpg	153.75	J/mol×K	471.61	Joback Method
cpg	162.24	J/mol×K	504.00	Joback Method
cpg	170.22	J/mol×K	536.40	Joback Method
cpg	177.72	J/mol×K	568.80	Joback Method
dvisc	0.0011217	Pa×s	213.98	Joback Method
dvisc	0.0008601	Pa×s	240.72	Joback Method
dvisc	0.0006954	Pa×s	267.46	Joback Method
dvisc	0.0005845	Pa×s	294.19	Joback Method
dvisc	0.0005056	Pa×s	320.93	Joback Method
dvisc	0.0004473	Pa×s	347.67	Joback Method
dvisc	0.0004027	Pa×s	374.41	Joback Method
hvapt	37.60	kJ/mol	374.00	NIST Webbook
hvapt	34.07	kJ/mol	384.40	NIST Webbook
pvap	102.18	kPa	385.00	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	89.62	kPa	380.60	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	80.03	kPa	376.90	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	70.04	kPa	372.60	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	59.85	kPa	367.60	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	49.78	kPa	362.10	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	40.07	kPa	355.60	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	30.05	kPa	347.70	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	20.07	kPa	337.00	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	9.95	kPa	320.80	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	6.06	kPa	310.10	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	3.65	kPa	300.00	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone:	https://www.doi.org/10.1021/acs.jced.7b00344
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C765435&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume