Ethanone, 1-(1-cyclohexen-1-yl)-

Other names:	Ketone, 1-cyclohexen-1-yl methyl
	Methyl 1-cyclohexenyl ketone
	1-Acetylcyclohexene
	1-Cyclohexen-1-yl methyl ketone
	1-Acetyl-1-cyclohexene
	1-[1-cyclohexen-1-yl]-ethanone
	cyclohex-1-enylmethylketone
Inchi:	InChI=1S/C8H12O/c1-7(9)8-5-3-2-4-6-8/h5H,2-4,6H2,1H3
InchiKey:	LTYLUDGDHUEBGX-UHFFFAOYSA-N
Formula:	C8H12O
SMILES:	CC(=O)C1=CCCCC1
Mol. weight [g/mol]:	124.18
CAS:	932-66-1

Physical Properties

Property code	Value	Unit	Source
gf	-59.95	kJ/mol	Joback Method
hf	-200.06	kJ/mol	Joback Method
hfus	9.67	kJ/mol	Joback Method
hvap	41.84	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.076		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	1023.00		NIST Webbook
tb	475.00 ± 7.00	K	NIST Webbook
tb	474.70	K	NIST Webbook
tc	681.88	K	Joback Method
tf	346.00	K	NIST Webbook
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.02	J/mol×K	464.67	Joback Method
cpg	237.48	J/mol×K	500.87	Joback Method
cpg	251.13	J/mol×K	537.07	Joback Method
cpg	263.98	J/mol×K	573.27	Joback Method
cpg	276.08	J/mol×K	609.48	Joback Method
cpg	287.44	J/mol×K	645.68	Joback Method
cpg	298.08	J/mol×K	681.88	Joback Method
dvisc	0.0044881	Pa×s	254.75	Joback Method
dvisc	0.0021682	Pa×s	289.74	Joback Method
dvisc	0.0012253	Pa×s	324.72	Joback Method
dvisc	0.0007737	Pa×s	359.71	Joback Method
dvisc	0.0005300	Pa×s	394.70	Joback Method
dvisc	0.0003862	Pa×s	429.68	Joback Method
dvisc	0.0002951	Pa×s	464.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	474.50 ± 0.50	K	2.70	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C932661&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume