Ethanone, 1-cyclohexyl-

Other names:	Ketone, cyclohexyl methyl
	Acetophenone, hexahydro-
	Acetylcyclohexane
	Cyclohexane, acetyl-
	Cyclohexyl methyl ketone
	Cyclohexylethanone
	Methyl cyclohexyl ketone
	1-Acetylcyclohexane
	c-C6H11COCH3
	NSC 16249
	1-Cyclohexylethanone
	1-cyclohexylethan-1-one
Inchi:	InChI=1S/C8H14O/c1-7(9)8-5-3-2-4-6-8/h8H,2-6H2,1H3
InchiKey:	RIFKADJTWUGDOV-UHFFFAOYSA-N
Formula:	C8H14O
SMILES:	CC(=O)C1CCCCC1
Mol. weight [g/mol]:	126.20
CAS:	823-76-7

Physical Properties

Property code	Value	Unit	Source
affp	841.40	kJ/mol	NIST Webbook
basg	809.50	kJ/mol	NIST Webbook
gf	-87.99	kJ/mol	Joback Method
hf	-266.71	kJ/mol	Joback Method
hfus	9.91	kJ/mol	Joback Method
hvap	40.58	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	2.156		Crippen Method
mcvol	114.290	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	963.00		NIST Webbook
rinpol	1007.00		NIST Webbook
tb	455.86	K	Joback Method
tc	669.17	K	Joback Method
tf	237.23	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.03	J/mol×K	455.86	Joback Method
cpg	254.60	J/mol×K	491.41	Joback Method
cpg	270.29	J/mol×K	526.96	Joback Method
cpg	285.12	J/mol×K	562.51	Joback Method
cpg	299.12	J/mol×K	598.06	Joback Method
cpg	312.30	J/mol×K	633.62	Joback Method
cpg	324.68	J/mol×K	669.17	Joback Method
dvisc	0.0059366	Pa×s	237.23	Joback Method
dvisc	0.0026543	Pa×s	273.67	Joback Method
dvisc	0.0014339	Pa×s	310.11	Joback Method
dvisc	0.0008817	Pa×s	346.55	Joback Method
dvisc	0.0005947	Pa×s	382.98	Joback Method
dvisc	0.0004296	Pa×s	419.42	Joback Method
dvisc	0.0003268	Pa×s	455.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.50 ± 0.50	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C823767&Units=SI

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

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

Legend

affp:	Proton affinity
basg:	Gas basicity
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