Ethanone, 1-(1-methylcyclohexyl)-

Other names:	1-(1-Methyl-cyclohexyl)-ethanone
	1-(1-Methyl-3-cyclohexen-3-yl)ethanol
Inchi:	InChI=1S/C9H16O/c1-8(10)9(2)6-4-3-5-7-9/h3-7H2,1-2H3
InchiKey:	UBMBCDFRVPGSSQ-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CC(=O)C1(C)CCCCC1
Mol. weight [g/mol]:	140.22
CAS:	2890-62-2

Physical Properties

Property code	Value	Unit	Source
gf	-85.06	kJ/mol	Joback Method
hf	-272.11	kJ/mol	Joback Method
hfus	6.20	kJ/mol	Joback Method
hvap	41.65	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.546		Crippen Method
mcvol	128.380	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	478.98	K	Joback Method
tc	698.54	K	Joback Method
tf	272.40	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.72	J/mol×K	478.98	Joback Method
cpg	300.39	J/mol×K	515.57	Joback Method
cpg	316.84	J/mol×K	552.17	Joback Method
cpg	332.21	J/mol×K	588.76	Joback Method
cpg	346.60	J/mol×K	625.35	Joback Method
cpg	360.13	J/mol×K	661.94	Joback Method
cpg	372.92	J/mol×K	698.54	Joback Method

hvapt	54.60	kJ/mol	384.00	NIST Webbook
hvapt	46.10	kJ/mol	394.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2890622&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

cpg:	Ideal gas heat capacity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume