Cyclopentanone, 3-methyl-

Other names:	3-Methyl-1-cyclopentanone
	3-Methylcyclopentanone
	DL-3-methylcyclopentanone
Inchi:	InChI=1S/C6H10O/c1-5-2-3-6(7)4-5/h5H,2-4H2,1H3
InchiKey:	AOKRXIIIYJGNNU-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CC1CCC(=O)C1
Mol. weight [g/mol]:	98.14
CAS:	1757-42-2

Physical Properties

Property code	Value	Unit	Source
chl	-3516.00	kJ/mol	NIST Webbook
ea	0.00 ± 0.00	eV	NIST Webbook
gf	-86.40	kJ/mol	Joback Method
hf	-244.39	kJ/mol	Joback Method
hfus	4.74	kJ/mol	Joback Method
hvap	33.45	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.375		Crippen Method
mcvol	86.110	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
rinpol	817.00		NIST Webbook
rinpol	847.50		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	858.00		NIST Webbook
rinpol	811.90		NIST Webbook
rinpol	847.60		NIST Webbook
rinpol	821.00		NIST Webbook
ripol	1225.00		NIST Webbook
ripol	1226.00		NIST Webbook
ripol	1218.00		NIST Webbook
tb	417.25 ± 0.40	K	NIST Webbook
tb	418.20	K	NIST Webbook

tc	637.42	K	Joback Method
tf	215.15 ± 3.00	K	NIST Webbook
tf	214.75 ± 0.40	K	NIST Webbook
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.13	J/mol×K	419.78	Joback Method
cpg	178.43	J/mol×K	456.05	Joback Method
cpg	191.20	J/mol×K	492.33	Joback Method
cpg	203.42	J/mol×K	528.60	Joback Method
cpg	215.09	J/mol×K	564.87	Joback Method
cpg	226.22	J/mol×K	601.15	Joback Method
cpg	236.80	J/mol×K	637.42	Joback Method

Sources

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=C1757422&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume