Cyclopentanone, 2-methyl-

Other names:	«alpha»-Methylcyclopentanone
	2-Methylcyclopentanone
	2-Methylcyclopentan-1-one
Inchi:	InChI=1S/C6H10O/c1-5-3-2-4-6(5)7/h5H,2-4H2,1H3
InchiKey:	ZIXLDMFVRPABBX-UHFFFAOYSA-N
Formula:	C6H10O
SMILES:	CC1CCCC1=O
Mol. weight [g/mol]:	98.14
CAS:	1120-72-5

Physical Properties

Property code	Value	Unit	Source
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	836.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	840.00		NIST Webbook
rinpol	848.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	842.90		NIST Webbook
rinpol	139.85		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	847.00		NIST Webbook
rinpol	139.85		NIST Webbook
rinpol	859.00		NIST Webbook
rinpol	848.00		NIST Webbook
ripol	1192.00		NIST Webbook

ripol	1177.00		NIST Webbook
ripol	1174.00		NIST Webbook
ripol	1177.00		NIST Webbook
ripol	1180.00		NIST Webbook
ripol	1167.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1220.00		NIST Webbook
ripol	1177.00		NIST Webbook
tb	412.70	K	NIST Webbook
tb	412.65 ± 0.70	K	NIST Webbook
tb	414.00 ± 4.00	K	NIST Webbook
tb	412.70 ± 0.50	K	NIST Webbook
tb	417.00 ± 6.00	K	NIST Webbook
tb	411.90 ± 2.00	K	NIST Webbook
tc	637.42	K	Joback Method
tf	197.05 ± 0.50	K	NIST Webbook
tf	198.15 ± 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=C1120725&Units=SI

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

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

Legend

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