Cyclohexanone, 4-methyl-

Other names:	4-Methylcyclohexanone
	p-Methyl cyclohexanone
	4-Methyl-1-cyclohexanone
	Methyl-4 cyclohexanone-1
Inchi:	InChI=1S/C7H12O/c1-6-2-4-7(8)5-3-6/h6H,2-5H2,1H3
InchiKey:	VGVHNLRUAMRIEW-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC1CCC(=O)CC1
Mol. weight [g/mol]:	112.17
CAS:	589-92-4

Physical Properties

Property code	Value	Unit	Source
affp	844.90	kJ/mol	NIST Webbook
basg	813.00	kJ/mol	NIST Webbook
ea	0.01 ± 0.00	eV	NIST Webbook
gf	-90.08	kJ/mol	Joback Method
hf	-271.19	kJ/mol	Joback Method
hfus	5.23	kJ/mol	Joback Method
hvap	35.85	kJ/mol	Joback Method
ie	9.16	eV	NIST Webbook
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	936.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	918.00		NIST Webbook

rinpol	943.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	954.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1348.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1342.00		NIST Webbook
tb	373.50 ± 1.00	K	NIST Webbook
tb	444.60 ± 0.60	K	NIST Webbook
tb	443.20	K	NIST Webbook
tc	670.65	K	Joback Method
tf	232.00 ± 5.00	K	NIST Webbook
tf	232.55 ± 0.50	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.80 ± 2.00	J/mol×K	490.00	NIST Webbook
cpg	206.20 ± 0.80	J/mol×K	445.00	NIST Webbook
cpg	211.30 ± 1.20	J/mol×K	450.00	NIST Webbook
cpg	215.70 ± 1.60	J/mol×K	460.00	NIST Webbook
cpg	218.80 ± 1.60	J/mol×K	470.00	NIST Webbook
cpg	221.80 ± 1.80	J/mol×K	480.00	NIST Webbook
cpg	227.80 ± 2.50	J/mol×K	500.00	NIST Webbook
cpl	207.10	J/mol×K	290.00	NIST Webbook
hvapt	45.30	kJ/mol	391.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C589924&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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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