

Cyclohexanone, 4-methyl-

Other names:	Methyl cyclohexanone methycyclohexanone
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:	1331-22-2

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mvol	100.200	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	438.20 ± 2.00	K	NIST Webbook
tc	670.65	K	Joback Method
tf	244.25	K	Joback Method
vc	0.367	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.07	J/mol×K	446.93	Joback Method
cpg	219.79	J/mol×K	484.22	Joback Method
cpg	234.85	J/mol×K	521.50	Joback Method
cpg	249.23	J/mol×K	558.79	Joback Method
cpg	262.92	J/mol×K	596.07	Joback Method
cpg	275.92	J/mol×K	633.36	Joback Method
cpg	288.21	J/mol×K	670.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1331222&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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