Cyclohexanone, 3-methyl-

Other names:	3-Methylcyclohexanone
	Methyl-3 cyclohexanone-1
Inchi:	InChI=1S/C7H12O/c1-6-3-2-4-7(8)5-6/h6H,2-5H2,1H3
InchiKey:	UJBOOUHRTQVGRU-UHFFFAOYSA-N
Formula:	C7H12O
SMILES:	CC1CCCC(=O)C1
Mol. weight [g/mol]:	112.17
CAS:	591-24-2

Physical Properties

Property code	Value	Unit	Source
chl	-4196.10	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
log10ws	-1.69		Crippen Method
logp	1.766		Crippen Method
mcvol	100.200	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
rinpol	924.00		NIST Webbook
rinpol	928.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	939.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	945.00		NIST Webbook

rinpol	915.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1333.00		NIST Webbook
ripol	1376.00		NIST Webbook
ripol	1376.00		NIST Webbook
tb	442.70	K	NIST Webbook
tb	442.70 ± 0.70	K	NIST Webbook
tc	670.65	K	Joback Method
tf	184.00 ± 6.00	K	NIST Webbook
tf	199.25 ± 0.50	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.92	J/mol×K	596.07	Joback Method
cpg	275.92	J/mol×K	633.36	Joback Method
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	288.21	J/mol×K	670.65	Joback Method
cpl	207.10	J/mol×K	290.00	NIST Webbook
hvapt	44.90	kJ/mol	387.50	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591242&Units=SI

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

Legend

chl:	Standard liquid enthalpy of combustion
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
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

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