Cyclohexanone,2-chloro-2-methyl-

Inchi: InChI=1S/C7H11ClO/c1-7(8)5-3-2-4-6(7)9/h2-5H2,1H3
InchiKey: IDRWHLQDVSLCBJ-UHFFFAOYSA-N
Formula: C7H11ClO
SMILES: CC1(Cl)CCCCC1=O
Mol. weight [g/mol]: 146.62
CAS: 10409-46-8

Physical Properties

Property code	Value	Unit	Source
gf	-107.50	kJ/mol	Joback Method
hf	-271.69	kJ/mol	Joback Method
hfus	3.13	kJ/mol	Joback Method
hvap	39.09	kJ/mol	Joback Method
ie	9.41	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.127		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	3708.97	kPa	Joback Method
tb	484.60	K	Joback Method
tc	725.07	K	Joback Method
tf	298.07	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.67	J/mol×K	484.60	Joback Method
cpg	247.83	J/mol×K	524.68	Joback Method
cpg	261.98	J/mol×K	564.76	Joback Method
cpg	275.23	J/mol×K	604.83	Joback Method
cpg	287.68	J/mol×K	644.91	Joback Method
cpg	299.46	J/mol×K	684.99	Joback Method
cpg	310.65	J/mol×K	725.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10409468&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

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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