Cyclohexanone, 2,6-dichloro

Inchi: InChI=1S/C6H8Cl2O/c7-4-2-1-3-5(8)6(4)9/h4-5H,1-3H2
InchiKey: MNOLFQQEONPNAT-UHFFFAOYSA-N
Formula: C6H8Cl2O
SMILES: O=C1C(Cl)CCCC1Cl
Mol. weight [g/mol]: 167.03

Physical Properties

Property code	Value	Unit	Source
gf	-130.07	kJ/mol	Joback Method
hf	-302.37	kJ/mol	Joback Method
hfus	12.11	kJ/mol	Joback Method
hvap	42.09	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.954		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
pc	3624.61	kPa	Joback Method
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	494.24	K	Joback Method
tc	733.96	K	Joback Method
tf	288.58	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.38	J/mol×K	494.24	Joback Method
cpg	231.12	J/mol×K	534.19	Joback Method
cpg	244.18	J/mol×K	574.15	Joback Method
cpg	256.55	J/mol×K	614.10	Joback Method
cpg	268.21	J/mol×K	654.05	Joback Method
cpg	279.13	J/mol×K	694.00	Joback Method
cpg	289.30	J/mol×K	733.96	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630701&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume