Cyclohexanone, 2,2-dichloro

Inchi: InChI=1S/C6H8Cl2O/c7-6(8)4-2-1-3-5(6)9/h1-4H2
InchiKey: AGFDSLIZRUCCKJ-UHFFFAOYSA-N
Formula: C6H8Cl2O
SMILES: O=C1CCCCC1(Cl)Cl
Mol. weight [g/mol]: 167.03

Physical Properties

Property code	Value	Unit	Source
gf	-127.85	kJ/mol	Joback Method
hf	-266.79	kJ/mol	Joback Method
hfus	4.74	kJ/mol	Joback Method
hvap	41.25	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.303		Crippen Method
mcvol	110.590	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
tb	499.15	K	Joback Method
tc	749.97	K	Joback Method
tf	316.72	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.17	J/mol×K	499.15	Joback Method
cpg	229.26	J/mol×K	540.95	Joback Method
cpg	241.39	J/mol×K	582.76	Joback Method
cpg	252.71	J/mol×K	624.56	Joback Method
cpg	263.32	J/mol×K	666.36	Joback Method
cpg	273.34	J/mol×K	708.16	Joback Method
cpg	282.89	J/mol×K	749.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630692&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
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