2-(Chloromethyl)cyclohexanone

Inchi: InChI=1S/C7H11ClO/c8-5-6-3-1-2-4-7(6)9/h6H,1-5H2
InchiKey: SITIRBGRZDHGGC-UHFFFAOYSA-N
Formula: C7H11ClO
SMILES: O=C1CCCCC1CCl
Mol. weight [g/mol]: 146.62

Physical Properties

Property code	Value	Unit	Source
gf	-102.01	kJ/mol	Joback Method
hf	-286.93	kJ/mol	Joback Method
hfus	9.43	kJ/mol	Joback Method
hvap	40.24	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.985		Crippen Method
mcvol	112.440	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
rinpol	1081.00		NIST Webbook
tb	484.36	K	Joback Method
tc	714.34	K	Joback Method
tf	274.17	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.26	J/mol×K	484.36	Joback Method
cpg	247.46	J/mol×K	522.69	Joback Method
cpg	261.93	J/mol×K	561.02	Joback Method
cpg	275.65	J/mol×K	599.35	Joback Method
cpg	288.63	J/mol×K	637.68	Joback Method
cpg	300.85	J/mol×K	676.01	Joback Method
cpg	312.31	J/mol×K	714.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R520580&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
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
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