1-Chloro-1-methylcyclohexane

Inchi: InChI=1S/C7H13Cl/c1-7(8)5-3-2-4-6-7/h2-6H2,1H3
InchiKey: OGYBTPYJHQSBBR-UHFFFAOYSA-N
Formula: C7H13Cl
SMILES: CC1(Cl)CCCCC1
Mol. weight [g/mol]: 132.63
CAS: 931-78-2

Physical Properties

Property code	Value	Unit	Source
gf	15.09	kJ/mol	Joback Method
hf	-133.99	kJ/mol	Joback Method
hfl	-246.00 ± 1.00	kJ/mol	NIST Webbook
hfus	3.62	kJ/mol	Joback Method
hvap	34.84	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.948		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
tb	394.00 ± 4.00	K	NIST Webbook
tc	637.44	K	Joback Method
tf	229.85	K	Joback Method
tt	234.52 ± 0.10	K	NIST Webbook
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.00	J/mol×K	600.66	Joback Method
cpg	203.95	J/mol×K	416.78	Joback Method
cpg	220.43	J/mol×K	453.56	Joback Method
cpg	235.66	J/mol×K	490.33	Joback Method
cpg	249.75	J/mol×K	527.11	Joback Method
cpg	262.83	J/mol×K	563.89	Joback Method
cpg	286.39	J/mol×K	637.44	Joback Method

hfust	1.63	kJ/mol	234.50	NIST Webbook

Sources

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=C931782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume