1,1,3-Trichlorocyclohexane

Inchi: InChI=1S/C6H9Cl3/c7-5-2-1-3-6(8,9)4-5/h5H,1-4H2
InchiKey: OYXGZLXUMFSCHC-UHFFFAOYSA-N
Formula: C6H9Cl3
SMILES: ClC1CCCC(Cl)(Cl)C1
Mol. weight [g/mol]: 187.50

Physical Properties

Property code	Value	Unit	Source
gf	-24.90	kJ/mol	Joback Method
hf	-165.17	kJ/mol	Joback Method
hfus	10.49	kJ/mol	Joback Method
hvap	41.07	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.342		Crippen Method
mcvol	121.260	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1143.00		NIST Webbook
tb	464.09	K	Joback Method
tc	702.00	K	Joback Method
tf	274.18	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	220.11	J/mol×K	464.09	Joback Method
cpg	233.87	J/mol×K	503.74	Joback Method
cpg	246.48	J/mol×K	543.39	Joback Method
cpg	258.06	J/mol×K	583.04	Joback Method

cpg	268.76	J/mol×K	622.70	Joback Method
cpg	278.72	J/mol×K	662.35	Joback Method
cpg	288.06	J/mol×K	702.00	Joback Method

Sources

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=R591498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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