1,1,2,2-Tetrachlorocyclohexane

Inchi: InChI=1S/C6H8Cl4/c7-5(8)3-1-2-4-6(5,9)10/h1-4H2
InchiKey: CVTKPHKRKFDAAO-UHFFFAOYSA-N
Formula: C6H8Cl4
SMILES: ClC1(Cl)CCCCC1(Cl)Cl
Mol. weight [g/mol]: 221.94

Physical Properties

Property code	Value	Unit	Source
gf	-42.32	kJ/mol	Joback Method
hf	-165.67	kJ/mol	Joback Method
hfus	8.39	kJ/mol	Joback Method
hvap	44.31	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.908		Crippen Method
mcvol	133.500	ml/mol	McGowan Method
pc	3543.08	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1272.00		NIST Webbook
tb	501.76	K	Joback Method
tc	756.73	K	Joback Method
tf	328.00	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.55	J/mol×K	501.76	Joback Method
cpg	257.89	J/mol×K	544.25	Joback Method
cpg	268.89	J/mol×K	586.75	Joback Method
cpg	278.84	J/mol×K	629.24	Joback Method
cpg	288.05	J/mol×K	671.74	Joback Method
cpg	296.84	J/mol×K	714.23	Joback Method
cpg	305.52	J/mol×K	756.73	Joback Method

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=R591572&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
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