1,1,3-trans-5-Tetrachlorocyclohexane

Inchi: InChI=1S/C6H8Cl4/c7-4-1-5(8)3-6(9,10)2-4/h4-5H,1-3H2/t4-,5-/m0/s1
InchiKey: INGHATHDMYGMDA-WHFBIAKZSA-N
Formula: C6H8Cl4
SMILES: ClC1CC(Cl)CC(Cl)(Cl)C1
Mol. weight [g/mol]: 221.94

Physical Properties

Property code	Value	Unit	Source
gf	-44.54	kJ/mol	Joback Method
hf	-201.25	kJ/mol	Joback Method
hfus	15.76	kJ/mol	Joback Method
hvap	45.15	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.559		Crippen Method
mcvol	133.500	ml/mol	McGowan Method
pc	3235.66	kPa	Joback Method
rinpol	1314.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1317.00		NIST Webbook
tb	496.85	K	Joback Method
tc	740.51	K	Joback Method
tf	299.86	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.89	J/mol×K	496.85	Joback Method
cpg	260.03	J/mol×K	537.46	Joback Method
cpg	272.09	J/mol×K	578.07	Joback Method
cpg	283.20	J/mol×K	618.68	Joback Method

cpg	293.52	J/mol×K	659.29	Joback Method
cpg	303.18	J/mol×K	699.90	Joback Method
cpg	312.33	J/mol×K	740.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R591423&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