1,1,2-trans-3-Tetrachlorocyclohexane

Inchi: InChI=1S/C6H8Cl4/c7-4-2-1-3-6(9,10)5(4)8/h4-5H,1-3H2/t4-,5+/m0/s1
InchiKey: DAPOKGIHMOAVTF-CRCLSJGQSA-N
Formula: C6H8Cl4
SMILES: ClC1CCCC(Cl)(Cl)C1Cl
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	1343.00		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1343.00		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

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=R591443&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