2,2,5-endo,6-exo,8b,8c,9c,10a-octachlorobornane

Inchi: InChI=1S/C10H10Cl8/c11-2-8(3-12)4-1-9(17,18)10(8,7(15)16)6(14)5(4)13/h4-7H,1-3H2/t
InchiKey: KYHLSFSZWAYDCA-KRMORPATSA-N
Formula: C10H10Cl8
SMILES: ClCC1(CCl)C2CC(Cl)(Cl)C1(C(Cl)Cl)C(Cl)C2Cl
Mol. weight [g/mol]: 413.81

Physical Properties

Property code	Value	Unit	Source
gf	-2.47	kJ/mol	Joback Method
hf	-277.13	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	67.86	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.663		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2373.20		NIST Webbook
tb	726.99	K	Joback Method
tc	988.40	K	Joback Method
tf	513.92	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.07	J/mol×K	726.99	Joback Method
cpg	520.99	J/mol×K	770.56	Joback Method
cpg	534.50	J/mol×K	814.13	Joback Method
cpg	549.15	J/mol×K	857.69	Joback Method
cpg	565.50	J/mol×K	901.26	Joback Method
cpg	584.12	J/mol×K	944.83	Joback Method
cpg	605.56	J/mol×K	988.40	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502448&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

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

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