

2,2,3-exo,5-endo,6-exo,8c,9b,10a-octachlorobornane

Inchi: InChI=1S/C10H10Cl8/c11-1-8(2-12)4-5(14)7(16)9(8,3-13)10(17,18)6(4)15/h4-7H,1-3H2/t
InchiKey: DHFLJTWYZQDYFD-OTDXBERWSA-N
Formula: C10H10Cl8
SMILES: ClC1(CCl)C2C(Cl)C(Cl)C1(CCl)C(Cl)(Cl)C2Cl
Mol. weight [g/mol]: 413.81

Physical Properties

Property code	Value	Unit	Source
gf	-7.74	kJ/mol	Joback Method
hf	-292.19	kJ/mol	Joback Method
hfus	35.86	kJ/mol	Joback Method
hvap	67.93	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.315		Crippen Method
mvol	227.960	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2352.10		NIST Webbook
rinpol	2352.10		NIST Webbook
tb	722.76	K	Joback Method
tc	979.11	K	Joback Method
tf	524.68	K	Joback Method
vc	0.882	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.18	J/mol×K	722.76	Joback Method
cpg	524.20	J/mol×K	765.48	Joback Method
cpg	537.70	J/mol×K	808.21	Joback Method
cpg	552.19	J/mol×K	850.93	Joback Method
cpg	568.20	J/mol×K	893.66	Joback Method
cpg	586.23	J/mol×K	936.38	Joback Method
cpg	606.80	J/mol×K	979.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R502379&Units=SI

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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