

2,2,5,5,9b,9c,10a,10b-octachlorobornane

Inchi:	InChI=1S/C10H10Cl8/c1-7-3-8(15,16)4(2-9(7,17)18)10(7,5(11)12)6(13)14/h4-6H,2-3H2,1
InchiKey:	QUDALMCYDIHOCE-UHFFFAOYSA-N
Formula:	C10H10Cl8
SMILES:	CC12CC(Cl)(Cl)C(CC1(Cl)Cl)C2(C(Cl)Cl)C(Cl)Cl
Mol. weight [g/mol]:	413.81

Physical Properties

Property code	Value	Unit	Source
gf	-2.69	kJ/mol	Joback Method
hf	-246.83	kJ/mol	Joback Method
hfus	20.38	kJ/mol	Joback Method
hvap	66.62	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	6.358		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinsol	2319.90		NIST Webbook
tb	731.46	K	Joback Method
tc	1008.58	K	Joback Method
tf	527.06	K	Joback Method
vc	0.871	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.15	J/mol×K	731.46	Joback Method
cpg	513.38	J/mol×K	777.65	Joback Method
cpg	528.08	J/mol×K	823.83	Joback Method
cpg	545.12	J/mol×K	870.02	Joback Method
cpg	565.36	J/mol×K	916.20	Joback Method
cpg	589.65	J/mol×K	962.39	Joback Method
cpg	618.87	J/mol×K	1008.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502413&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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