

2,2,5,5,8c,9b,10a,10b-octachlorobornane

Inchi:	InChI=1S/C10H10Cl8/c11-3-7-2-9(15,16)5(1-10(7,17)18)8(7,4-12)6(13)14/h5-6H,1-4H2
InchiKey:	ITMIBUSOOSKJOV-UHFFFAOYSA-N
Formula:	C10H10Cl8
SMILES:	C1CC1(C(CI)CI)C2CC(CI)(CI)C1(CCI)CC2(CI)CI
Mol. weight [g/mol]:	413.81

Physical Properties

Property code	Value	Unit	Source
gf	-0.25	kJ/mol	Joback Method
hf	-241.55	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	67.01	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	6.012		Crippen Method
mcvol	227.960	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinsol	2423.80		NIST Webbook
tb	731.90	K	Joback Method
tc	1003.15	K	Joback Method
tf	542.06	K	Joback Method
vc	0.876	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	499.53	J/mol×K	731.90	Joback Method
cpg	512.46	J/mol×K	777.11	Joback Method
cpg	526.82	J/mol×K	822.32	Joback Method
cpg	543.41	J/mol×K	867.52	Joback Method
cpg	563.03	J/mol×K	912.73	Joback Method
cpg	586.50	J/mol×K	957.94	Joback Method
cpg	614.62	J/mol×K	1003.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502399&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
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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