

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

lnChI=1S/C10H8Cl10/c11-2-7-4(12)10(19,20)3(1-8(7,17)18)9(7,5(13)14)6(15)16/h3-6H,1

MDVFGNFJNPTVIP-BJPUCQMRS-A-N

C10H8Cl10

C1CC12C(Cl)C(Cl)(Cl)C(CC1(Cl)Cl)C2(C(Cl)Cl)C(Cl)Cl

482.70

Physical Properties

Property code	Value	Unit	Source
gf	-34.26	kJ/mol	Joback Method
hf	-298.65	kJ/mol	Joback Method
hfus	29.84	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.794		Crippen Method
mcvol	252.440	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2685.00		NIST Webbook
tb	801.65	K	Joback Method
tc	1081.26	K	Joback Method
tf	582.66	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.27	J/mol×K	801.65	Joback Method
cpg	561.79	J/mol×K	848.25	Joback Method
cpg	580.09	J/mol×K	894.85	Joback Method
cpg	602.07	J/mol×K	941.46	Joback Method
cpg	628.60	J/mol×K	988.06	Joback Method
cpg	660.55	J/mol×K	1034.66	Joback Method
cpg	698.80	J/mol×K	1081.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R502384&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
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
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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