P-chloro-n-(2,3,4,4,5,6-hexachloro-2,5-cyclohexad

Inchi: InChI=1S/C12H4Cl7N/c13-5-1-3-6(4-2-5)20-9-7(14)10(16)12(18,19)11(17)8(9)15/h1-4H
InchiKey: CBJDZZJVHXDKQX-UHFFFAOYSA-N
Formula: C12H4Cl7N
SMILES: ClC1=C(Cl)C(Cl)(Cl)C(Cl)=C(Cl)C1=Nc1ccc(Cl)cc1
Mol. weight [g/mol]: 410.34

Physical Properties

Property code	Value	Unit	Source
hf	4.14	kJ/mol	Joback Method
hvap	82.59	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.978		Crippen Method
mcvol	228.080	ml/mol	McGowan Method
pc	2106.13	kPa	Joback Method
tb	884.82	K	Joback Method
tc	1170.25	K	Joback Method

Sources

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=B6001832&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature