# 2,2',4,4',5,5'-Hexachloro azobenzene

**Inchi:** InChI=1S/C12H4Cl6N2/c13-5-1-9(17)11(3-7(5)15)19-20-12-4-8(16)6(14)2-10(12)18/h1-4
**InchiKey:** SMDPHUIHCPMCKV-FMQUCBEESA-N
**Formula:** C12H4Cl6N2
**SMILES:** Clc1cc(Cl)c(N=Nc2cc(Cl)c(Cl)cc2Cl)cc1Cl
**Mol. weight [g/mol]:** 388.89
**CAS:** 25016-08-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | 66.01 | kJ/mol | Joback Method |
| hvap | 83.81 | kJ/mol | Joback Method |
| log10ws | -7.62 | | Crippen Method |
| logp | 8.022 | | Crippen Method |
| mcvol | 221.520 | ml/mol | McGowan Method |
| pc | 1920.30 | kPa | Joback Method |
| tb | 930.98 | K | Joback Method |
| tc | 1212.48 | K | Joback Method |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C25016084&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

## 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 |