4,6,7-trichloro-2,1,3-benzothiadiazole

Inchi: InChI=1S/C6HCl3N2S/c7-2-1-3(8)5-6(4(2)9)11-12-10-5/h1H
InchiKey: SZYWFOPNFNROQB-UHFFFAOYSA-N
Formula: C6HCl3N2S
SMILES: Clc1cc(Cl)c2nsnc2c1Cl
Mol. weight [g/mol]: 239.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Aqueous Solubility Prediction Method
logp	3.652		Crippen Method
mcvol	129.510	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume