chlorquinox

Other names: 5,6,7,8-Tetrachloroquinoxaline
Inchi: InChI=1S/C8H2Cl4N2/c9-3-4(10)6(12)8-7(5(3)11)13-1-2-14-8/h1-2H
InchiKey: NHTGQOXRZFUGJX-UHFFFAOYSA-N
Formula: C8H2Cl4N2
SMILES: Clc1c(Cl)c(Cl)c2nccnc2c1Cl
Mol. weight [g/mol]: 267.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Aqueous Solubility Prediction Method
log10ws	-5.43		Estimated Solubility Method
logp	4.243		Crippen Method
mcvol	149.280	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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