6-Chloro-2-methyl-7-methylsulfamyl-benzothiatria

Inchi: InChI=1S/C8H9ClN4O4S2/c1-10-18(14,15)7-4-8-6(3-5(7)9)11-12-13(2)19(8,16)17/h3-4,1
InchiKey: PZTXTWSLFNUDLW-UHFFFAOYSA-N
Formula: C8H9ClN4O4S2
SMILES: CNS(=O)(=O)c1cc2c(cc1Cl)N=NN(C)S2(=O)=O
Mol. weight [g/mol]: 324.76
CAS: 1917-30-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	0.881		Crippen Method
mcvol	193.000	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1917302&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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