6-Chloro-2-methyl-7-sulfamyl-3,4-dihydro-1,2,4-be

Inchi: InChI=1S/C8H10ClN3O4S2/c1-12-4-11-6-2-5(9)7(17(10,13)14)3-8(6)18(12,15)16/h2-3,1
InchiKey: CNSCONHVBQJXDB-UHFFFAOYSA-N
Formula: C8H10ClN3O4S2
SMILES: CN1CNc2cc(Cl)c(S(N)(=O)=O)cc2S1(=O)=O
Mol. weight [g/mol]: 311.77
CAS: 90606-97-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.51		Crippen Method
logp	-0.009		Crippen Method
mcvol	187.320	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90606976&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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