sulfamethizole

Other names: 4-Amino-N-(5-methyl-1,3,4-thiadiazol-2-yl)benzenesulfonamide
Inchi: InChI=1S/C9H10N4O2S2/c1-6-11-12-9(16-6)13-17(14,15)8-4-2-7(10)3-5-8/h2-5H,10H2,1
InchiKey: VACCAVUAMIDAGB-UHFFFAOYSA-N
Formula: C9H10N4O2S2
SMILES: Cc1nnc(NS(=O)(=O)c2ccc(N)cc2)s1
Mol. weight [g/mol]: 270.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.71		Aqueous Solubility Prediction Method
log10ws	-2.78		Aqueous Solubility Prediction Method
logp	1.230		Crippen Method
mcvol	178.810	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
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/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