sulfapyrazine

Inchi: InChI=1S/C10H10N4O2S/c11-8-1-3-9(4-2-8)17(15,16)14-10-7-12-5-6-13-10/h1-7H,11H2
InchiKey: YEAICDDXRUOCKJ-UHFFFAOYSA-N
Formula: C10H10N4O2S
SMILES: Nc1ccc(S(=O)(=O)Nc2cnccn2)cc1
Mol. weight [g/mol]: 250.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Aqueous Solubility Prediction Method
logp	0.860		Crippen Method
mcvol	172.250	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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

Legend

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