4-(3-hydroxyphenyl)sulfonylthiophene-2-sulfonam

Inchi: InChI=1S/C10H9NO5S3/c11-19(15,16)10-5-9(6-17-10)18(13,14)8-3-1-2-7(12)4-8/h1-6,12
InchiKey: LRQUYRADZABVMX-UHFFFAOYSA-N
Formula: C10H9NO5S3
SMILES: NS(=O)(=O)c1cc(S(=O)(=O)c2cccc(O)c2)cs1
Mol. weight [g/mol]: 319.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.72		Aqueous Solubility Prediction Method
logp	0.934		Crippen Method
mcvol	196.920	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
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