

4-(4-hydroxyphenyl)sulfonylthiophene-2-sulfonamide

Inchi: InChI=1S/C10H9NO5S3/c11-19(15,16)10-5-9(6-17-10)18(13,14)8-3-1-7(12)2-4-8/h1-6,12
InchiKey: IGEMDIAQXSOCKX-UHFFFAOYSA-N
Formula: C10H9NO5S3
SMILES: NS(=O)(=O)c1cc(S(=O)(=O)c2ccc(O)cc2)cs1
Mol. weight [g/mol]: 319.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.03		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/ci9903071>
Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
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

Latest version available from:

<https://www.cheméo.com/cid/112-482-2/4-4-hydroxyphenyl-sulfonylthiophene-2-sulfonamide.pdf>

Generated by Cheméo on 2024-05-02 23:10:57.497027187 +0000 UTC m=+16980706.417604509.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.