4-(4-methoxyphenyl)sulfonylthiophene-2-sulfonar

Inchi: InChI=1S/C11H11NO5S3/c1-17-8-2-4-9(5-3-8)19(13,14)10-6-11(18-7-10)20(12,15)16/h2
InchiKey: VDAMAZDKFJYVCT-UHFFFAOYSA-N
Formula: C11H11NO5S3
SMILES: COc1ccc(S(=O)(=O)c2csc(S(N)(=O)=O)c2)cc1
Mol. weight [g/mol]: 333.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.22		Aqueous Solubility Prediction Method
logp	1.237		Crippen Method
mcvol	211.010	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