4-(4-methoxybenzoyl)thiophene-2-sulfonamide

Inchi: InChI=1S/C12H11NO4S2/c1-17-10-4-2-8(3-5-10)12(14)9-6-11(18-7-9)19(13,15)16/h2-7H
InchiKey: CNGDZXAWOIPFFX-UHFFFAOYSA-N
Formula: C12H11NO4S2
SMILES: COc1ccc(C(=O)c2csc(S(N)(=O)=O)c2)cc1
Mol. weight [g/mol]: 297.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.47		Aqueous Solubility Prediction Method
logp	1.635		Crippen Method
mcvol	198.580	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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