4-(4-methylbenzoyl)thiophene-2-sulfonamide

Inchi: InChI=1S/C12H11NO3S2/c1-8-2-4-9(5-3-8)12(14)10-6-11(17-7-10)18(13,15)16/h2-7H,1H
InchiKey: GYTMHWVFKHLDEA-UHFFFAOYSA-N
Formula: C12H11NO3S2
SMILES: Cc1ccc(C(=O)c2csc(S(N)(=O)=O)c2)cc1
Mol. weight [g/mol]: 281.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Aqueous Solubility Prediction Method
logp	1.935		Crippen Method
mcvol	192.710	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