4-amino-N-(4-methyl-1,3-thiazol-2-yl)benzenesulfo

Inchi: InChI=1S/C10H11N3O2S2/c1-7-6-16-10(12-7)13-17(14,15)9-4-2-8(11)3-5-9/h2-6H,11H2
InchiKey: KJVQYDYPDFFJMP-UHFFFAOYSA-N
Formula: C10H11N3O2S2
SMILES: Cc1csc(NS(=O)(=O)c2ccc(N)cc2)n1
Mol. weight [g/mol]: 269.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Aqueous Solubility Prediction Method
logp	1.835		Crippen Method
mcvol	182.920	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