

# 4-(4-methoxyphenyl)sulfonylthiophene-2-sulfonamide

<b>Inchi:</b>	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
<b>InchiKey:</b>	VDAMAZDKFJYVCT-UHFFFAOYSA-N
<b>Formula:</b>	C11H11NO5S3
<b>SMILES:</b>	COc1ccc(S(=O)(=O)c2csc(S(N)(=O)=O)c2)cc1
<b>Mol. weight [g/mol]:</b>	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

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/112-029-5/4-4-methoxyphenyl-sulfonylthiophene-2-sulfonamide.pdf>

Generated by Cheméo on 2024-05-02 21:25:55.985425334 +0000 UTC m=+16974404.906002650.

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