

4-(4-hydroxyphenyl)sulfonylfuran-2-sulfonamide

Inchi:	InChI=1S/C10H9NO6S2/c11-19(15,16)10-5-9(6-17-10)18(13,14)8-3-1-7(12)2-4-8/h1-6,12
InchiKey:	NKPDCGFEJUINIK-UHFFFAOYSA-N
Formula:	C10H9NO6S2
SMILES:	NS(=O)(=O)c1cc(S(=O)(=O)c2ccc(O)cc2)co1
Mol. weight [g/mol]:	303.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Aqueous Solubility Prediction Method
logp	0.465		Crippen Method
mcvol	186.440	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
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

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