

sulfapyrazine

Inchi: InChI=1S/C10H10N4O2S/c11-8-1-3-9(4-2-8)17(15,16)14-10-7-12-5-6-13-10/h1-7H,11H2
InchiKey: YEAI CDDXR UOCKJ-UHFFFAOYSA-N
Formula: C10H10N4O2S
SMILES: Nc1ccc(S(=O)(=O)Nc2cnccn2)cc1
Mol. weight [g/mol]: 250.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Aqueous Solubility Prediction Method
logp	0.860		Crippen Method
mcvol	172.250	ml/mol	McGowan Method

Sources

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

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/100-720-0/sulfapyrazine.pdf>

Generated by Cheméo on 2024-04-23 19:45:19.975496864 +0000 UTC m=+16190768.896074174.

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