

2-methylsulfanylpteridine

Inchi:	InChI=1S/C7H6N4S/c1-12-7-10-4-5-6(11-7)9-3-2-8-5/h2-4H,1H3
InchiKey:	LNTLWEUAGAFRJR-UHFFFAOYSA-N
Formula:	C7H6N4S
SMILES:	CSc1ncc2nccnc2n1
Mol. weight [g/mol]:	178.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Aqueous Solubility Prediction Method
logp	1.142		Crippen Method
mcvol	122.540	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/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

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