4-methylsulfanylpteridine

Inchi: InChI=1S/C7H6N4S/c1-12-7-5-6(10-4-11-7)9-3-2-8-5/h2-4H,1H3
InchiKey: XKENOTHGZDIXRS-UHFFFAOYSA-N
Formula: C7H6N4S
SMILES: CSc1ncnc2nccnc12
Mol. weight [g/mol]: 178.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.36		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/ci990307l
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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