1H-pteridine-2-thione

Inchi: InChI=1S/C6H4N4S/c11-6-9-3-4-5(10-6)8-2-1-7-4/h1-3H,(H,8,9,10,11)
InchiKey: DAAQPMSPBHQGQA-UHFFFAOYSA-N
Formula: C6H4N4S
SMILES: S=c1ncc2nccnc2[nH]1
Mol. weight [g/mol]: 164.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Aqueous Solubility Prediction Method
logp	0.600		Crippen Method
mcvol	108.450	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/ci990307l
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