

# 1H-pteridine-2-thione

<b>Inchi:</b>	InChI=1S/C6H4N4S/c11-6-9-3-4-5(10-6)8-2-1-7-4/h1-3H,(H,8,9,10,11)
<b>InchiKey:</b>	DAAQPMSPBHQQQA-UHFFFAOYSA-N
<b>Formula:</b>	C6H4N4S
<b>SMILES:</b>	S=c1ncc2nccnc2[nH]1
<b>Mol. weight [g/mol]:</b>	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/ci9903071>

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

## Legend

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

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