

Pteridine

Inchi: InChI=1S/C6H4N4/c1-2-9-6-5(8-1)3-7-4-10-6/h1-4H
InchiKey: CPNGPNLZQNNVQM-UHFFFAOYSA-N
Formula: C6H4N4
SMILES: c1cnc2ncncc2n1
Mol. weight [g/mol]: 132.13

Physical Properties

Property code	Value	Unit	Source
log10ws	0.02		Aqueous Solubility Prediction Method
log10ws	0.02		Estimated Solubility Method
logp	0.420		Crippen Method
mcvol	92.100	ml/mol	McGowan Method
tf	412.65	K	Aqueous Solubility Prediction Method

Sources

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

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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<https://www.cheméo.com/cid/112-182-5/Pteridine.pdf>

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