

4-Pteridinamine, N,N-dimethyl-

Other names: N,N-dimethylpteridin-4-amine
Inchi: InChI=1S/C8H9N5/c1-13(2)8-6-7(11-5-12-8)10-4-3-9-6/h3-5H,1-2H3
InchiKey: KXQWQYBKUMVBIB-UHFFFAOYSA-N
Formula: C8H9N5
SMILES: CN(C)c1ncnc2nccnc12
Mol. weight [g/mol]: 175.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.02		Aqueous Solubility Prediction Method
log10ws	-1.02		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.486		Crippen Method
mcvol	130.260	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>

Aqueous and cosolvent solubility data for drug-like organic compounds: <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>

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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