N,N-dimethylpteridin-2-amine

Inchi: InChI=1S/C8H9N5/c1-13(2)8-11-5-6-7(12-8)10-4-3-9-6/h3-5H,1-2H3
InchiKey: JXKUCNDDDQEMSS-UHFFFAOYSA-N
Formula: C8H9N5
SMILES: CN(C)c1ncc2nccnc2n1
Mol. weight [g/mol]: 175.20

Physical Properties

Property code	Value	Unit	Source
log10ws	0.36		Aqueous Solubility Prediction Method
log10ws	0.36		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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.