4-Pteridinamine

Inchi: InChI=1S/C6H5N5/c7-5-4-6(11-3-10-5)9-2-1-8-4/h1-3H,(H2,7,9,10,11)
InchiKey: VFATYAVSACUHHG-UHFFFAOYSA-N
Formula: C6H5N5
SMILES: Nc1ncnc2nccnc12
Mol. weight [g/mol]: 147.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.002		Crippen Method
mcvol	102.080	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 and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/

Legend

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