

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/ci9903071
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

Latest version available from:

<https://www.cheméo.com/cid/105-158-0/4-Pteridinamine.pdf>

Generated by Cheméo on 2024-04-29 21:26:54.351630894 +0000 UTC m=+16715263.272208209.

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