

pteridin-7-amine

Inchi:	InChI=1S/C6H5N5/c7-5-2-9-4-1-8-3-10-6(4)11-5/h1-3H,(H2,7,8,10,11)
InchiKey:	KJVGXOHRFWZQJB-UHFFFAOYSA-N
Formula:	C6H5N5
SMILES:	Nc1cnc2cncnc2n1
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

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/
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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