

6-Methylpteridine

Inchi:	InChI=1S/C7H6N4/c1-5-2-9-7-6(11-5)3-8-4-10-7/h2-4H,1H3
InchiKey:	IQCHKMQERZPOIJ-UHFFFAOYSA-N
Formula:	C7H6N4
SMILES:	Cc1cnc2ncncc2n1
Mol. weight [g/mol]:	146.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.14		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	0.728		Crippen Method
mcvol	106.190	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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