

Pteridine, 2-amino-6,7-dimethyl-

Inchi:	InChI=1S/C8H9N5/c1-4-5(2)12-7-6(11-4)3-10-8(9)13-7/h3H,1-2H3,(H2,9,10,12,13)
InchiKey:	QDEJQTTZZROSHU-UHFFFAOYSA-N
Formula:	C8H9N5
SMILES:	Cc1nc2cnc(N)nc2nc1C
Mol. weight [g/mol]:	175.19
CAS:	19153-00-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	0.619		Crippen Method
mcvol	130.260	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19153005&Units=SI

Legend

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

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