

4(1H)-Pteridinone, 2-amino-

Other names:	Pteridoxamine Pterin Quinonoid dihydropterin, 2-amino- 2-Amino-4(1H)-pteridinone 2-Amino-4(3H)-pteridinone 2-Amino-4-hydroxypteridine 2-Amino-4-pteridone 4-Oxopterin Pterine 2-Amino-4-oxopterin NSC 11540 NSC 170929 NSC 18696 2-amino-1H-pteridin-4-one
Inchi:	InChI=1S/C6H5N5O/c7-6-10-4-3(5(12)11-6)8-1-2-9-4/h1-2H,(H3,7,9,10,11,12)
InchiKey:	HNXQXTQTPAJEJL-UHFFFAOYSA-N
Formula:	C6H5N5O
SMILES:	<chem>N=c1nc(O)c2nccnc2[nH]1</chem>
Mol. weight [g/mol]:	163.14
CAS:	2236-60-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.33		Crippen Method
logp	-0.944		Crippen Method
mvol	107.950	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2236604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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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