

Pterin-6-carboxylic acid

Other names:	Pterine-6-carboxylic acid 2-Amino-4-hydroxypteridine-6-carboxylic acid 6-Pteridinecarboxylic acid, 2-amino-1,4-dihydro-4-oxo- 2-amino-1,4-dihydro-4-oxopteridine-6-carboxylic acid
Inchi:	InChI=1S/C7H5N5O3/c8-7-11-4-3(5(13)12-7)10-2(1-9-4)6(14)15/h1H,(H,14,15)(H3,8,9,1
InchiKey:	QABAUCFGPWONOG-UHFFFAOYSA-N
Formula:	C7H5N5O3
SMILES:	<chem>Nc1nc2ncc(C(=O)O)nc2c(=O)[nH]1</chem>
Mol. weight [g/mol]:	207.15
CAS:	948-60-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	-1.488		Crippen Method
mcvol	129.480	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C948607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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