

4-Amino-2,6-dihydroxypyrimidine

Other names:	6-Amino-2,4-dihydroxypyrimidine 6-Aminouracil 4-Aminouracil 2,4(1H,3H)-Pyrimidinedione, 6-amino- Cytosine, 6-hydroxy- Uracil, 6-amino- 4-Amino-2,6-dihydroxypyrimidine 4-Amino-2,6-dioxypyrimidine 4-Amino-2,6-pyrimidinediol 6-Amino-2,4-pyrimidinediol 2,4-Dihydroxy-6-aminopyrimidine 6-Amino-1H-pyrimidine-2,4-dione NSC 15919 NSC 7367
Inchi:	InChI=1S/C4H5N3O2/c5-2-1-3(8)7-4(9)6-2/h1H,(H4,5,6,7,8,9)
InchiKey:	LNDZXOWGUAUIUBG-UHFFFAOYSA-N
Formula:	C4H5N3O2
SMILES:	<chem>Nc1cc(=O)[nH]c(=O)[nH]1</chem>
Mol. weight [g/mol]:	127.10
CAS:	873-83-6

Physical Properties

Property code	Value	Unit	Source
log10ws	1.61		Crippen Method
logp	-2.318		Crippen Method
mcvol	85.140	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=C873836&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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