

4-amino-2-hydroxypyrimidine

Other names:	2(1H)-pyrimidinone, 4-amino- 4-amino-2(1H)-pyrimidinone cytosine cytosinimine
Inchi:	InChI=1S/C4H5N3O/c5-3-1-2-6-4(8)7-3/h1-2H,(H3,5,6,7,8)
InchiKey:	OPTASPLRGRRNAP-UHFFFAOYSA-N
Formula:	C4H5N3O
SMILES:	<chem>Nc1cc[nH]c(=O)n1</chem>
Mol. weight [g/mol]:	111.10

Physical Properties

Property code	Value	Unit	Source
log10ws	0.49		Crippen Method
logp	-1.130		Crippen Method
mcvol	79.270	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric interaction coefficients for some nucleosides in aqueous solution	https://www.doi.org/10.1016/j.jct.2012.12.014
Viscometric studies on nucleic acid bases and nucleosides in aqueous solution	https://www.doi.org/10.1016/j.jct.2014.10.015
Swelling behavior of nucleosides at T _m and T _m - 10 K in water and deuterium oxide	https://www.doi.org/10.1016/j.jct.2015.11.029
McGowan Method	http://link.springer.com/article/10.1007/BF02311772
hydrochloride solutions: Viscometric, calorimetric and spectroscopic approach:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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