

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 <https://www.doi.org/10.1016/j.jct.2012.12.014>

Yotum et al. studies on nucleic acid <https://www.doi.org/10.1016/j.jct.2014.10.015>

bases and nucleosides in aqueous <https://www.doi.org/10.1016/j.jct.2015.11.029>

Guar gum hydrochloride solutions at T <https://www.doi.org/10.1016/j.jct.2015.11.029>

acq bases and nucleosides in water <http://link.springer.com/article/10.1007/BF02311772>

and deoxyribose in water <http://link.springer.com/article/10.1007/BF02311772>

hydrochloride solutions: Viscometric, <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

calorimetric and spectroscopic <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

approach:

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/64-259-4/4-amino-2-hydroxypyrimidine.pdf>

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