4-amino-2-hydroxypyrimidine

Other names: 2(1H)-pyrimidinone, 4-amino-

4-amino-2(1H)-pyrimidinone

cytosine

cytosinimine

InChl=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: Nc1cc[nH]c(=O)n1

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

Solvation behavior of some nucleic acid bases and nucleosides in water McGiovanu Matte glianidine hydrochloride solutions: Viscometric, calbane let and spectroscopic

approach: Crippen Method:

Volumetric interaction coefficients for some nucleosides in aqueous solution youngelgics kudies on nucleic acid bases and nucleosides in aqueous guanidine hydrochloride solutions at T = (288.15 to 318.15) K and at atmospheric pressure:

https://www.doi.org/10.1016/j.jct.2015.11.029

http://link.springer.com/article/10.1007/BF02311772

http://pubs.acs.org/doi/abs/10.1021/ci990307l

https://www.chemeo.com/doc/models/crippen_log10ws

https://www.doi.org/10.1016/j.jct.2012.12.014 https://www.doi.org/10.1016/j.jct.2014.10.015

Legend

log10ws:Log10 of Water solubility in mol/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volume

Latest version available from:

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

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