2(1H)-Pyrimidinone, 4-amino-

Other names:	4-Amino-2(1H)pyrimidone
	4-Amino-2-oxypyrimidine
	4-amino-2(1H)-pyrimidinone
	4-amino-2-hydroxypyrimidine
	Cyt
	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:	Nc1cc[nH]c(=O)n1
Mol. weight [g/mol]:	111.10

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.15		Cheméo Relay (1.0)
logp	-1.130		Crippen Method
mcvol	79.270	ml/mol	McGowan Method
tf	607.00	K	Melting temperature and heat of fusion of cytosine revealed from fast scanning calorimetry

Sources

Volumetric interaction coefficients for some nucleosides in aqueous solution at T = 288.15 K:	https://www.doi.org/10.1016/j.jct.2012.12.014
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric studies 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.2014.10.015
Melting temperature and heat of fusion of cytosine revealed from fast scanning calorimetry:	https://www.doi.org/10.1016/j.tca.2017.09.013
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C71307&Units=SI
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solvation behavior of some nucleic acid bases and nucleosides in water and in aqueous guanidine hydrochloride solutions: Viscometric, calorimetric and spectroscopic approach:	https://www.doi.org/10.1016/j.jct.2015.11.029
Crippen Method:	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
tf:	Normal melting (fusion) point