

2(1H)-Pyrimidinone, 4-amino-5-methyl-

Other names:	Cytosine, 5-methyl- 5-Methylcytosine
Inchi:	InChI=1S/C5H7N3O/c1-3-2-7-5(9)8-4(3)6/h2H,1H3,(H3,6,7,8,9)
InchiKey:	LRSASMSXMSNRBT-UHFFFAOYSA-N
Formula:	C5H7N3O
SMILES:	Cc1cnc(O)nc1N
Mol. weight [g/mol]:	125.13
CAS:	554-01-8

Physical Properties

Property code	Value	Unit	Source
ie	8.78	eV	NIST Webbook
log10ws	-0.66		Crippen Method
logp	0.073		Crippen Method
mcvol	93.360	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C554018&Units=SI

Legend

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

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