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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