

# 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:** Cc1c[nH]c(=O)nc1N  
**Mol. weight [g/mol]:** 125.13

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.56		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-1.46		Aqueous Solubility Prediction Method
log10ws	-1.46		Estimated Solubility Method
logp	-0.821		Crippen Method
mcvol	93.360	ml/mol	McGowan Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

**Aqueous and cosolvent solubility data for drug-like organic compounds:** <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/>

## Legend

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

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