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)[nH]c1N
Mol. weight [g/mol]: 125.13

Physical Properties

Property code	Value	Unit	Source
hf	-138.09	kJ/mol	Cheméo Relay (1.0)
ie	8.67	eV	Cheméo Relay (1.0)
log10ws	-1.46		Aqueous Solubility Prediction Method
log10ws	-1.46		Estimated Solubility Method
log10ws	-0.56		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.821		Crippen Method
mcvol	93.360	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
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
Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf: Enthalpy of formation at standard conditions

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