5-Fluorocytosine

Inchi: InChI=1S/C4H4FN3O/c5-2-1-7-4(9)8-3(2)6/h1H,(H3,6,7,8,9)
InchiKey: XRECTZIEBJDKEO-UHFFFAOYSA-N
Formula: C4H4FN3O
SMILES: Nc1[nH]c(=O)ncc1F
Mol. weight [g/mol]: 129.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.05		Aqueous Solubility Prediction Method
log10ws	-0.96		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	-0.991		Crippen Method
mcvol	81.040	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/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.