2(1H)Pyrimidinone,1-methyl-

Other names: 1,2-Dihydropyrimidin-2-one, 1-methyl-
Inchi: InChI=1S/C5H6N2O/c1-7-4-2-3-6-5(7)8/h2-4H,1H3
InchiKey: LQKMCBPMBNUKSU-UHFFFAOYSA-N
Formula: C5H6N2O
SMILES: Cn1cccnc1=O
Mol. weight [g/mol]: 110.11
CAS: 3739-81-9

Physical Properties

Property code	Value	Unit	Source
ie	9.31 ± 0.05	eV	NIST Webbook
log10ws	-1.95		Crippen Method
logp	-0.220		Crippen Method
mcvol	83.380	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=C3739819&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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