Pyridine, 1-acetyl-1,2,3,4-tetrahydro-

Other names: 1-Acetyl-1,2,3,4-tetrahydropyridine
Inchi: InChI=1S/C7H11NO/c1-7(9)8-5-3-2-4-6-8/h3,5H,2,4,6H2,1H3
InchiKey: ZGKNRILGBQAZDJ-UHFFFAOYSA-N
Formula: C7H11NO
SMILES: CC(=O)N1C=CCCC1
Mol. weight [g/mol]: 125.17
CAS: 19615-27-1

Physical Properties

Property code	Value	Unit	Source
ie	8.80	eV	NIST Webbook
log10ws	-1.34		Crippen Method
logp	1.142		Crippen Method
mcvol	105.880	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=C19615271&Units=SI

Legend

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