

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/ci9903071
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

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<https://www.chemeo.com/cid/36-183-9/Pyridine-1-acetyl-1-2-3-4-tetrahydro.pdf>

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