

4(H)-Pyridine, N-acetyl-

Other names:	N-Acetyl-4H-pyridine
Inchi:	InChI=1S/C7H9NO/c1-7(9)8-5-3-2-4-6-8/h3-6H,2H2,1H3
InchiKey:	YPZBIQKYSOYOGV-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	CC(=O)N1C=CCC=C1
Mol. weight [g/mol]:	123.15
CAS:	67402-83-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.69		Crippen Method
logp	1.266		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
rinpol	1038.00		NIST Webbook
rinpol	1038.00		NIST Webbook

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=C67402839&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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