3-Pyridinol, 4-methyl-, acetate (ester)

Other names: 3-Acetoxy-4-methylpyridine
Inchi: InChI=1S/C8H9NO2/c1-6-3-4-9-5-8(6)11-7(2)10/h3-5H,1-2H3
InchiKey: JLIFSYCXGJGLGE-UHFFFAOYSA-N
Formula: C8H9NO2
SMILES: CC(=O)Oc1cnccc1C
Mol. weight [g/mol]: 151.16
CAS: 1006-96-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	1.315		Crippen Method
mcvol	117.240	ml/mol	McGowan Method
ripol	1897.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1006968&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
ripol: Polar retention indices