3-Pyridinol, 6-methyl-, acetate (ester)

Other names:	2-Methyl-5-acetoxypyridine
	5-Acetoxy-2-methylpyridine
	5-Acetoxy-2-picoline
Inchi:	InChI=1S/C8H9NO2/c1-6-3-4-8(5-9-6)11-7(2)10/h3-5H,1-2H3
InchiKey:	WXLRJJLUBRXUPX-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	CC(=O)Oc1ccc(C)nc1
Mol. weight [g/mol]:	151.16
CAS:	4842-89-1

Physical Properties

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

Sources

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=C4842891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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