

4-Pyridinol, acetate (ester)

Other names:	4-Acetoxy pyridine 4-pyridinyl acetate
Inchi:	InChI=1S/C7H7NO2/c1-6(9)10-7-2-4-8-5-3-7/h2-5H,1H3
InchiKey:	PTZQTYADHHANGW-UHFFFAOYSA-N
Formula:	C7H7NO2
SMILES:	CC(=O)Oc1ccncc1
Mol. weight [g/mol]:	137.14
CAS:	14210-20-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	1.007		Crippen Method
mcvol	103.150	ml/mol	McGowan Method
ripol	1643.00		NIST Webbook
ripol	1643.00		NIST Webbook

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=C14210209&Units=SI

Legend

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

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