3-(2-pyridyl)propyl acetate

Other names:	2-Pyridinepropanol, acetate (ester)
	Pyridine, 2-(3-acetoxypropyl)-
Inchi:	InChI=1S/C10H13NO2/c1-9(12)13-8-4-6-10-5-2-3-7-11-10/h2-3,5,7H,4,6,8H2,1H3
InchiKey:	WJNAEONVLSWDTG-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CC(=O)OCCCc1ccccn1
Mol. weight [g/mol]:	179.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	1.577		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
rinpol	1414.00		NIST Webbook

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=U372996&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
rinpol:	Non-polar retention indices

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