Pyridine, 1-acetyl-5-(1-acetyl-2-piperidinyl)-1,2,3,4-tetrahydr

Other names: N-Acetylammodendrine
Inchi: InChI=1S/C14H22N2O2/c1-11(17)15-8-5-6-13(10-15)14-7-3-4-9-16(14)12(2)18/h10,14H,
InchiKey: AITYIJXYFMGTNF-UHFFFAOYSA-N
Formula: C14H22N2O2
SMILES: CC(=O)N1C=C(C2CCCCN2C(C)=O)CCC1
Mol. weight [g/mol]: 250.34
CAS: 54966-21-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	1.914		Crippen Method
mcvol	205.200	ml/mol	McGowan Method
rinpol	2220.00		NIST Webbook
rinpol	2220.00		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=C54966211&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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