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

Other names: N-Formylammodendrine
Inchi: InChI=1S/C13H20N2O2/c1-11(17)14-8-4-5-12(9-14)13-6-2-3-7-15(13)10-16/h9-10,13H,2
InchiKey: IDRBUUNZHYXUPN-UHFFFAOYSA-N
Formula: C13H20N2O2
SMILES: CC(=O)N1C=C(C2CCCCN2C=O)CCC1
Mol. weight [g/mol]: 236.31
CAS: 54966-16-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	1.523		Crippen Method
mcvol	191.110	ml/mol	McGowan Method
rinpol	2222.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2222.00		NIST Webbook
rinpol	2210.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54966164&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices