

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

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/ci9903071
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

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