

# 2,3'-Bipyridine, 1'-acetyl-1',3,4,4',5,5',6,6'-octahydro-

Other names:	N-Acetylhystrine
Inchi:	InChI=1S/C12H18N2O/c1-10(15)14-8-4-5-11(9-14)12-6-2-3-7-13-12/h9H,2-8H2,1H3
InchiKey:	VGALILHZAQZXRBUHFFFAOYSA-N
Formula:	C12H18N2O
SMILES:	CC(=O)N1C=C(C2=NCCCC2)CCC1
Mol. weight [g/mol]:	206.28
CAS:	52195-93-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.49		Crippen Method
logp	2.137		Crippen Method
mcvol	171.150	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1932.00		NIST Webbook

## Sources

NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C52195934&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52195934&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## 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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