

Pyridine, 3-(3,4-dihydro-2H-pyrrol-5-yl)-

Other names:	Pyridine, 3-(1-pyrrolin-2-yl)- Myosmine 2-(3-Pyridyl)-1-pyrroline Miosmine
Inchi:	InChI=1S/C9H10N2/c1-3-8(7-10-5-1)9-4-2-6-11-9/h1,3,5,7H,2,4,6H2
InchiKey:	DPNGWXJMIILTBS-UHFFFAOYSA-N
Formula:	C9H10N2
SMILES:	<chem>c1cncc(C2=NCCC2)c1</chem>
Mol. weight [g/mol]:	146.19
CAS:	532-12-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.664		Crippen Method
mcvol	118.710	ml/mol	McGowan Method
rinpole	1427.30		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C532127&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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