Nicotyrine

Other names:	Pyridine, 3-(1-methyl-1H-pyrrol-2-yl)-
	Pyridine, 3-(1-methylpyrrol-2-yl)-
	«beta»-Nicotyrine
	1-Methyl-2-(3-pyridyl)pyrrole
	3-(1-Methyl-2-pyrrolyl)pyridine
	3,2'-Nicotyrine
	Pyridine, 3-(1-methyl-2-pyrrolyl)-
	3-(1-Methyl-1H-pyrrol-2-yl)pyridine
	NSC 127943
	3-(1-methylpyrrol-2-yl)pyridine
Inchi:	InChI=1S/C10H10N2/c1-12-7-3-5-10(12)9-4-2-6-11-8-9/h2-8H,1H3
InchiKey:	RYFOJXFXERAMLS-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	Cn1cccc1-c1cccnc1
Mol. weight [g/mol]:	158.20
CAS:	487-19-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.13		Crippen Method
logp	2.087		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
rinpol	1488.40		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C487194&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices