

Nicotine, 1'-demethyl-, (.+/-.)-

Other names:	(.+/-.)-1'-Demethylnicotine (.+/-.)-Nornicotine «beta»-dl-Nornicotine (R,S)-Nornicotine Pyridine, 3-(2-pyrrolidinyl)-, (.+/-.)- DI-nornicotine
Inchi:	InChI=1S/C9H12N2/c1-3-8(7-10-5-1)9-4-2-6-11-9/h1,3,5,7,9,11H,2,4,6H2
InchiKey:	MYKUKUCHPMASKF-UHFFFAOYSA-N
Formula:	C9H12N2
SMILES:	<chem>c1cncc(C2CCCN2)c1</chem>
Mol. weight [g/mol]:	148.21
CAS:	5746-86-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.42		Crippen Method
logp	1.506		Crippen Method
mcpol	123.010	ml/mol	McGowan Method
rinpol	1435.40		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C494973&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/12-239-3/Nicotine-1-demethyl.pdf>

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