Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, 1-oxide, (S)-

Other names:	Nicotine, 1-oxide
	Nicotine N-oxide
	Nicotine 1-N-oxide
	Nikotin-N-oxyd
Inchi:	InChI=1S/C10H14N2O/c1-11-6-3-5-10(11)9-4-2-7-12(13)8-9/h2,4,7-8,10H,3,5-6H2,1H3
InchiKey:	YHXKVHQFWVYXIC-UHFFFAOYSA-N
Formula:	C10H14N2O
SMILES:	CN1CCCC1c1ccc[n+]([O-])c1
Mol. weight [g/mol]:	178.23
CAS:	2820-55-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	1.087		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
rinpol	1477.80		NIST Webbook
rinpol	1477.80		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2820555&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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