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