Nornicotine

Other names:	Pyridine, 3-(2-pyrrolidinyl)-, (S)-
	Nicotine, 1'-demethyl-, (S)-
	(S)-2-(3-Pyridyl)pyrrolidine
	Nornicotin
	(S)-(-)-Nornicotine
	2-(3-Pyridyl)pyrrolidine
	l-Nor-nicotine
	3-(2-Pyrrolidinyl)pyridine
	(S)-Nornicotine
	Pyridine, 3-(2S)-2-pyrrolidinyl-
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/t9-/m0/s1
InchiKey:	MYKUKUCHPMASKF-VIFPVBQESA-N
Formula:	C9H12N2
SMILES:	c1cncc(C2CCCN2)c1
Mol. weight [g/mol]:	148.21
CAS:	494-97-3

Physical Properties

Property code	Value	Unit	Source
affp	964.00	kJ/mol	NIST Webbook
basg	931.00	kJ/mol	NIST Webbook
log10ws	-2.42		Crippen Method
logp	1.506		Crippen Method
mcvol	123.010	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.70	K	1.50	NIST Webbook

Sources

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

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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