

N-Nitrosornicotine

Other names:	Nornicotine, N-nitroso
Inchi:	InChI=1S/C9H11N3O/c13-11-12-6-2-4-9(12)8-3-1-5-10-7-8/h1,3,5,7,9H,2,4,6H2
InchiKey:	XKABJYQDMJTNGQ-UHFFFAOYSA-N
Formula:	C9H11N3O
SMILES:	O=NN1CCCC1c1cccnc1
Mol. weight [g/mol]:	177.20
CAS:	16543-55-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	1.900		Crippen Method
mcvol	134.560	ml/mol	McGowan Method

Sources

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=C16543558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/97-127-4/N-Nitrosornicotine.pdf>

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