

Nornicotine, N-formyl

Inchi:	InChI=1S/C10H12N2O/c13-8-12-6-2-4-10(12)9-3-1-5-11-7-9/h1,3,5,7-8,10H,2,4,6H2
InchiKey:	GQLSEYOOXBRDFZ-UHFFFAOYSA-N
Formula:	C10H12N2O
SMILES:	O=CN1CCCC1c1cccnc1
Mol. weight [g/mol]:	176.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	1.375		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
rinpole	1783.00		NIST Webbook
rinpole	1783.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R44825&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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