

Carbamic acid, dimethyl-, 3-pyridinyl ester

Other names:	3-Pyridyl dimethylcarbamate Norpyridostigmine Carbamic acid, dimethyl-, 3-pyridyl ester Carbamic acid, dimethyl-, 3-pyridinyl ester (from Pyridostigmine bromide)
Inchi:	InChI=1S/C8H10N2O2/c1-10(2)8(11)12-7-4-3-5-9-6-7/h3-6H,1-2H3
InchiKey:	VZELUFSMNDBCBO-UHFFFAOYSA-N
Formula:	C8H10N2O2
SMILES:	CN(C)C(=O)Oc1cccnc1
Mol. weight [g/mol]:	166.18
CAS:	51581-32-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Crippen Method
logp	1.142		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
rinpol	1515.00		NIST Webbook
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Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C51581329&Units=SI

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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