Arecoline

Other names: 1,2,5,6-Tetrahydro-1-methyl-3-pyridinecarboxylic acid methyl ester
1,2,5,6-Tetrahydro-1-methylnicotinic acid, methyl ester
1-methyl-1,2,5,6-tetrahydro-pyridine-3-carboxylic acid methyl ester
3-Pyridinecarboxylic acid, 1,2,5,6-tetrahydro-1-methyl-, methyl ester
Arecaidine methyl ester
Arecaline
Arecholine
Arecolin
Arecoline base
Arekolin
Methyl 1,2,5,6-tetrahydro-1-methylnicotinate
Methyl N-methyl-1,2,5,6-tetrahydronicotinate
Methyl N-methyltetrahydronicotinate
Methylarecaiden
Methylarecaidine
N-Methyl-«delta»-tetrahydronicotinic acid methyl ester
N-Methyl-Â«deltaÂ»-tetrahydronicotinic acid methyl ester
N-Methyltetrahydronicotinic acid, methyl ester
N-Methyltetrahydropyridine-«beta»-carboxylic acid methyl ester
N-Methyltetrahydropyridine-Â«betaÂ»-carboxylic acid methyl ester
NSC 56321
Nicotinic acid, 1,2,5,6-tetrahydro-1-methyl-, methyl ester

Inchi: InChI=1S/C8H13NO2/c1-9-5-3-4-7(6-9)8(10)11-2/h4H,3,5-6H2,1-2H3

InchiKey: HJJPJSXJAXAIPN-UHFFFAOYSA-N

Formula: C8H13NO2

SMILES: COC(=O)C1=CCCN(C)C1

Mol. weight [g/mol]: 155.19

CAS: 63-75-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.81		Aqueous Solubility Prediction Method
logp	0.421		Crippen Method
mcvol	125.840	ml/mol	McGowan Method
rinpol	1195.00		NIST Webbook
rinpol	1236.10		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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