

Nicotinic acid, 1,2-dihydro-4,6-dimethyl-2-oxo-,ethyl ester

Inchi:	InChI=1S/C10H13NO3/c1-4-14-10(13)8-6(2)5-7(3)11-9(8)12/h5H,4H2,1-3H3,(H,11,12)
InchiKey:	GZBUMXFWJBMWEE-UHFFFAOYSA-N
Formula:	C10H13NO3
SMILES:	CCOC(=O)c1c(C)cc(C)nc1O
Mol. weight [g/mol]:	195.22
CAS:	16108-48-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	1.581		Crippen Method
mcvol	151.290	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16108488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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

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