

Nicotinic acid, 2,2-dimethylpropyl ester

Inchi:	InChI=1S/C11H15NO2/c1-11(2,3)8-14-10(13)9-5-4-6-12-7-9/h4-7H,8H2,1-3H3
InchiKey:	HACBDVGSFXLCDK-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CC(C)(C)COC(=O)c1cccnc1
Mol. weight [g/mol]:	193.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.284		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
rinpola	1382.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308333&Units=SI
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

Legend

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

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