

# Nicotinic acid, 1-cyclopentylethyl ester

**Inchi:** InChI=1S/C13H17NO2/c1-10(11-5-2-3-6-11)16-13(15)12-7-4-8-14-9-12/h4,7-11H,2-3,5-6  
**InchiKey:** KLONXUOFUMPOCQ-UHFFFAOYSA-N  
**Formula:** C13H17NO2  
**SMILES:** CC(OC(=O)c1cccnc1)C1CCCC1  
**Mol. weight [g/mol]:** 219.28

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	2.817		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
rinpole	1679.00		NIST Webbook
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## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308367&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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  
**rinpole:** Non-polar retention indices

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