

# Isonicotinic acid, 1-cyclopentylethyl ester

**Inchi:** InChI=1S/C13H17NO2/c1-10(11-4-2-3-5-11)16-13(15)12-6-8-14-9-7-12/h6-11H,2-5H2,1H  
**InchiKey:** MHNKRHAAQLYXQE-UHFFFAOYSA-N  
**Formula:** C13H17NO2  
**SMILES:** CC(OC(=O)c1ccncc1)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
rinpola	1661.00		NIST Webbook

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U308361&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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