

# Nicotinic acid, (4-chlorophenyl)methyl ester

**Inchi:** InChI=1S/C13H10ClNO2/c14-12-5-3-10(4-6-12)9-17-13(16)11-2-1-7-15-8-11/h1-8H,9H2  
**InchiKey:** FLUZHFKASOGKOP-UHFFFAOYSA-N  
**Formula:** C13H10ClNO2  
**SMILES:** O=C(OCc1ccc(Cl)cc1)c1cccnc1  
**Mol. weight [g/mol]:** 247.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	3.092		Crippen Method
mcvol	176.170	ml/mol	McGowan Method
rinsol	1972.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=U308352&Units=SI>

## Legend

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

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