

# Nicotinic acid, 3-phenylpropyl ester

**Inchi:** InChI=1S/C15H15NO2/c17-15(14-9-4-10-16-12-14)18-11-5-8-13-6-2-1-3-7-13/h1-4,6-7,9  
**InchiKey:** IJXNGPWCHMAWGL-UHFFFAOYSA-N  
**Formula:** C15H15NO2  
**SMILES:** O=C(OCCCc1ccccc1)c1cccnc1  
**Mol. weight [g/mol]:** 241.29

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.871		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
rinsol	1990.00		NIST Webbook
rinsol	1990.00		NIST Webbook

## Sources

**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>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U308370&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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