

# Isonicotinic acid, nonyl ester

**Inchi:** InChI=1S/C15H23NO2/c1-2-3-4-5-6-7-8-13-18-15(17)14-9-11-16-12-10-14/h9-12H,2-8,1  
**InchiKey:** LNSLZFGNVRHPJG-UHFFFAOYSA-N  
**Formula:** C15H23NO2  
**SMILES:** CCCCCCCCOC(=O)c1ccncc1  
**Mol. weight [g/mol]:** 249.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.989		Crippen Method
mcvol	215.870	ml/mol	McGowan Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		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=U299964&Units=SI>

## Legend

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

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