

# Isonicotinic acid, dodecyl ester

**Inchi:** InChI=1S/C18H29NO2/c1-2-3-4-5-6-7-8-9-10-11-16-21-18(20)17-12-14-19-15-13-17/h12  
**InchiKey:** AHDVQERFCJZEAX-UHFFFAOYSA-N  
**Formula:** C18H29NO2  
**SMILES:** CCCCCCCCCCOC(=O)c1ccncc1  
**Mol. weight [g/mol]:** 291.43

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.08		Crippen Method
logp	5.159		Crippen Method
mcvol	258.140	ml/mol	McGowan Method

## 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=U299887&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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