

# Nicotinic acid, dodec-9-ynyl ester

**Inchi:** InChI=1S/C18H25NO2/c1-2-3-4-5-6-7-8-9-10-11-15-21-18(20)17-13-12-14-19-16-17/h12  
**InchiKey:** KCGGZBGJNHLAAM-UHFFFAOYSA-N  
**Formula:** C18H25NO2  
**SMILES:** CCC#CCCCCCCCOC(=O)c1cccnc1  
**Mol. weight [g/mol]:** 287.40

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	4.383		Crippen Method
mcvol	249.540	ml/mol	McGowan Method
rinpol	2261.00		NIST Webbook
rinpol	2261.00		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=U299976&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/65-302-4/Nicotinic-acid-dodec-9-ynyl-ester.pdf>

Generated by Cheméo on 2024-04-27 03:50:41.636491686 +0000 UTC m=+16479090.557068998.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.