

# Nicotinic acid, undecyl ester

**Inchi:** InChI=1S/C17H27NO2/c1-2-3-4-5-6-7-8-9-10-14-20-17(19)16-12-11-13-18-15-16/h11-13  
**InchiKey:** OWEZDQWMGDOLFG-UHFFFAOYSA-N  
**Formula:** C17H27NO2  
**SMILES:** CCCCCCCCCCOC(=O)c1cccnc1  
**Mol. weight [g/mol]:** 277.40

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.67   |        | Crippen Method |
| logp          | 4.769   |        | Crippen Method |
| mcvol         | 244.050 | ml/mol | McGowan Method |
| rinpola       | 2121.00 |        | NIST Webbook   |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U299975&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/58-352-7/Nicotinic-acid-undecyl-ester.pdf>

Generated by Cheméo on 2024-04-27 03:58:57.512579758 +0000 UTC m=+16479586.433157103.

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