

# Isonipecotic acid, N-ethoxycarbonyl-, hexadecyl ester

**Inchi:** InChI=1S/C25H47NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-30-24(27)23-18-20-2  
**InchiKey:** KZAKLDZDHISVBE-UHFFFAOYSA-N  
**Formula:** C25H47NO4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC)CC1  
**Mol. weight [g/mol]:** 425.64

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.21		Crippen Method
logp	6.879		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpol	3324.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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=U322014&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

Latest version available from:

<https://www.chemeo.com/cid/14-370-5/Isonipecotic-acid-N-ethoxycarbonyl-hexadecyl-ester.pdf>

Generated by Cheméo on 2024-04-29 09:42:45.021585486 +0000 UTC m=+16673013.942162801.

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