

# Isonipecotic acid, N-isobutoxycarbonyl-, pentadecyl ester

**Inchi:** InChI=1S/C26H49NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-21-30-25(28)24-17-19-27(2)  
**InchiKey:** ANEMABVLDIFMEN-UHFFFAOYSA-N  
**Formula:** C26H49NO4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC(C)C)CC1  
**Mol. weight [g/mol]:** 439.67

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.39		Crippen Method
logp	7.125		Crippen Method
mcvol	391.200	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=U322073&Units=SI>

## Legend

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

Latest version available from:

<https://www.cheméo.com/cid/61-466-7/Isonipecotic-acid-N-isobutoxycarbonyl-pentadecyl-ester.pdf>

Generated by Cheméo on 2024-04-25 21:00:08.268779673 +0000 UTC m=+16368057.189356983.

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