

# Isonipecotic acid, N-methoxycarbonyl-, tetradecyl ester

**Inchi:** InChI=1S/C22H41NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-19-27-21(24)20-15-17-23(18-16)  
**InchiKey:** LFGDXUSTJXCDHQ-UHFFFAOYSA-N  
**Formula:** C22H41NO4  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OC)CC1  
**Mol. weight [g/mol]:** 383.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.96		Crippen Method
logp	5.709		Crippen Method
mcvol	334.840	ml/mol	McGowan Method
rinpola	2862.00		NIST Webbook
rinpola	2862.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322029&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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

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