

# Isonipecotic acid, N-ethohycarbonyl-, pentadecyl ester

**Inchi:** InChI=1S/C24H45NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-21-29-23(26)22-17-19-25(2)  
**InchiKey:** QQQXXISCGQWYSY-UHFFFAOYSA-N  
**Formula:** C24H45NO4  
**SMILES:** CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)OCC)CC1  
**Mol. weight [g/mol]:** 411.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	6.489		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
rinpole	3105.00		NIST Webbook
rinpole	3105.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322013&Units=SI>  
**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)

## Legend

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

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