

# Isonipecotic acid, N-(octanoyl)-, undecyl ester

**Inchi:** InChI=1S/C25H47NO3/c1-3-5-7-9-10-11-12-14-16-22-29-25(28)23-18-20-26(21-19-23)2  
**InchiKey:** YZEISMRKDDHYHJ-UHFFFAOYSA-N  
**Formula:** C25H47NO3  
**SMILES:** CCCCCCCCCCOC(=O)C1CCN(C(=O)CCCCCCC)CC1  
**Mol. weight [g/mol]:** 409.65

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.15		Crippen Method
logp	6.659		Crippen Method
mcvol	371.240	ml/mol	McGowan Method
rinpola	3186.00		NIST Webbook

## Sources

**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=U361577&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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