

# Isonipecotic acid, N-(4-methylbenzoyl)-, undecyl ester

**Inchi:** InChI=1S/C25H39NO3/c1-3-4-5-6-7-8-9-10-11-20-29-25(28)23-16-18-26(19-17-23)24(27)  
**InchiKey:** DMMXUEIOESQOSY-UHFFFAOYSA-N  
**Formula:** C25H39NO3  
**SMILES:** CCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C)cc2)CC1  
**Mol. weight [g/mol]:** 401.58

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.89		Crippen Method
logp	5.921		Crippen Method
mcvol	347.480	ml/mol	McGowan Method
rinpole	3329.00		NIST Webbook
rinpole	3329.00		NIST Webbook

## 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=U361123&Units=SI>

## 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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