

# Isonipecotic acid, N-(3-fluorobenzoyl)-, tetradecyl ester

**Inchi:** InChI=1S/C27H42FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-21-32-27(31)23-17-19-29(20-18)  
**InchiKey:** IDWDLWFTRFNQNH-UHFFFAOYSA-N  
**Formula:** C27H42FNO3  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1  
**Mol. weight [g/mol]:** 447.63

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.00		Crippen Method
logp	6.922		Crippen Method
mcvol	377.430	ml/mol	McGowan Method
rinsol	3486.00		NIST Webbook
rinsol	3486.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361530&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  
**rinsol:** Non-polar retention indices

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