

# Isonipectic acid, N-(3-fluorobenzoyl)-, dodecyl ester

**Inchi:** InChI=1S/C25H38FNO3/c1-2-3-4-5-6-7-8-9-10-11-19-30-25(29)21-15-17-27(18-16-21)24  
**InchiKey:** NYMAHWVAUQFVEU-UHFFFAOYSA-N  
**Formula:** C25H38FNO3  
**SMILES:** CCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1  
**Mol. weight [g/mol]:** 419.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	6.142		Crippen Method
mcvol	349.250	ml/mol	McGowan Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		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=U361528&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  
**rinpol:** Non-polar retention indices

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