

# Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, pentadecyl ester

InChI: InChI=1S/C29H43F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-37-28(36)23-15-17-34(16-18)O1  
InChIKey: STAXFUJHEIYZTA-UHFFFAOYSA-N

**Formula:** C<sub>29</sub>H<sub>43</sub>F<sub>4</sub>NO<sub>3</sub>  
**SMILES:** CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1  
**Mol. weight [g/mol]:** 529.65

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.52		Crippen Method
logp	8.331		Crippen Method
mcvol	410.920	ml/mol	McGowan Method
rinpole	3344.00		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=U361459&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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