

# Isonipecotic acid, N-(2-trifluoromethylbenzoyl)-, tridecyl ester

**Inchi:** InChI=1S/C27H40F3NO3/c1-2-3-4-5-6-7-8-9-10-11-14-21-34-26(33)22-17-19-31(20-18-2  
**InchiKey:** YHXNLGLSIGYQBK-UHFFFAOYSA-N  
**Formula:** C27H40F3NO3  
**SMILES:** CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2C(F)(F)F)CC1  
**Mol. weight [g/mol]:** 483.61

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	7.412		Crippen Method
mcvol	380.970	ml/mol	McGowan Method
rinpola	3314.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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=U361498&Units=SI>

## 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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