

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

InChI: InChI=1S/C30H45F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-38-29(37)24-16-18-3  
InChIKey: HGJGTUBYLJTKDS-UHFFFAOYSA-N

Formula: C30H45F4NO3

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]: 543.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.94		Crippen Method
logp	8.721		Crippen Method
mcvol	425.010	ml/mol	McGowan Method
rropol	3456.00		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=U361460&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
- rropol:** Non-polar retention indices

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