

# Isonipecotic acid, N-(2-fluoro-5-trifluoromethylbenzoyl)-, hexadecyl ester

InChI: InChI=1S/C30H45F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-38-29(37)24-18-20-3  
InChIKey: MNIAYSVDLPMHTJ-UHFFFAOYSA-N

Formula: C30H45F4NO3  
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)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
rinpol	3530.00		NIST Webbook
rinpol	3530.00		NIST Webbook

## Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>  
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361401&Units=SI>  
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
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  
rinpol: Non-polar retention indices

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