

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

InChI: InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-36-27(35)22-16-18-33(19-14-15)/q1  
InChIKey: IEXVPPSGLOGSKY-UHFFFAOYSA-N

Formula: C28H41F4NO3  
SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)CC1  
Mol. weight [g/mol]: 515.62

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.10		Crippen Method
logp	7.941		Crippen Method
mcvol	396.830	ml/mol	McGowan Method
rinpola	3303.00		NIST Webbook

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361399&Units=SI>  
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
Crippen Method: [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)  
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

## 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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