

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

InChI: InChI=1S/C26H37F4NO3/c1-2-3-4-5-6-7-8-9-10-11-16-34-25(33)20-12-14-31(15-13-20)2  
InChIKey: KHJIGUXNNNRQMS-UHFFFAOYSA-N

Formula: C26H37F4NO3

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

Mol. weight [g/mol]: 487.57

## Physical Properties

Property code	Value	Unit	Source
log10ws	-8.26		Crippen Method
logp	7.161		Crippen Method
mcvol	368.650	ml/mol	McGowan Method
rinpol	3043.00		NIST Webbook
rinpol	3043.00		NIST Webbook

## Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361456&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)

## 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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