

# L-Proline, N-(3-fluoro-5-trifluoromethylbenzoyl)-, tetradecyl ester

InChI: CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)cc(C(F)(F)F)c1  
InChIKey: ITSZFDDMOHDCCOC-UHFFFAOYSA-N

Formula: C<sub>27</sub>H<sub>39</sub>F<sub>4</sub>NO<sub>3</sub>

SMILES: CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 501.60

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.04		Crippen Method
logp	7.693		Crippen Method
mcvol	382.740	ml/mol	McGowan Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook

## Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345957&Units=SI>

## 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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