

# L-Proline, N-(3-fluoro-4-trifluoromethylbenzoyl)-, heptadecyl ester

InChI: InChI=1S/C30H45F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-38-29(37)27-18-1  
InChIKey: NLWSQZKNWLVMHC-UHFFFAOYSA-N

**Formula:** C30H45F4NO3  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(C(F)(F)F)c(F)c1  
**Mol. weight [g/mol]:** 543.68

## Physical Properties

Property code	Value	Unit	Source
log10ws	-10.29		Crippen Method
logp	8.864		Crippen Method
mcvol	425.010	ml/mol	McGowan Method
rinpol	3471.00		NIST Webbook
rinpol	3471.00		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=U345974&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  
**rinpol:** Non-polar retention indices

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