

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

**Inchi:** InChI=1S/C30H46F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-37-29(36)27-21-1  
**InchiKey:** MOEBNQRPHBTROY-UHFFFAOYSA-N  
**Formula:** C30H46F3NO3  
**SMILES:** CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1  
**Mol. weight [g/mol]:** 525.69

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.96		Crippen Method
logp	8.725		Crippen Method
mcvol	423.240	ml/mol	McGowan Method
rinpol	3472.00		NIST Webbook
rinpol	3472.00		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=U346353&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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