

# L-Proline, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, hexadecyl ester

InChI: InChI=1S/C29H44F3NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-37-29(35)24-18-17  
InChIKey: HQFVTPMGFPAKHB-UHFFFAOYSA-N

Formula: C29H44F3NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 527.66

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.55		Crippen Method
logp	7.742		Crippen Method
mcvol	415.020	ml/mol	McGowan Method
rinpol	3545.00		NIST Webbook
rinpol	3545.00		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=U346032&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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