L-Proline, N-(3-trifluoromethylbenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C28H42F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-35-27(34)25-19-16-20-3

InchiKey: SVRKKOMWDVLGMW-UHFFFAOYSA-N

Formula: C28H42F3NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 497.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.12		Crippen Method
logp	7.944		Crippen Method
mcvol	395.060	ml/mol	McGowan Method
rinpol	3260.00		NIST Webbook
rinpol	3260.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346351&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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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