

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

InChI: InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-36-27(35)25-16-15-17-3
InChIKey: INJGFKRAGFGNTQ-UHFFFAOYSA-N

Formula: C28H41F4NO3
SMILES: CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 515.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.45		Crippen Method
logp	8.084		Crippen Method
mcvol	396.830	ml/mol	McGowan Method
rinpol	3148.00		NIST Webbook
rinpol	3148.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: 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=U345958&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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