

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

InChI: InChI=1S/C31H47F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-39-30(38)28-1
InChIKey: DUSFCZMNFUOEKO-UHFFFAOYSA-N

Formula: C₃₁H₄₇F₄NO₃

SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)cc(C(F)(F)F)c1

Mol. weight [g/mol]: 557.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.71		Crippen Method
logp	9.254		Crippen Method
mcvol	439.100	ml/mol	McGowan Method
rinpole	3503.00		NIST Webbook
rinpole	3503.00		NIST Webbook

Sources

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

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

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345961&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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