L-Proline, N-(2-fluoro-3-trifluoromethylbenzoyl)-, octadecyl ester

Inchi: InChI=1S/C31H47F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-39-30(38)27-2
InchiKey: XRJNRRLDZCGDJN-UHFFFAOYSA-N
Formula: C31H47F4NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1F
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
rinpol	3577.00		NIST Webbook
rinpol	3577.00		NIST Webbook

Sources

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=U346005&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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