

L-Proline, N-(2-fluoro-5-trifluoromethylbenzoyl)-, heptadecyl ester

InChI: InChI=1S/C30H45F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-38-29(37)27-18-19-20-21
InChIKey: NCJIPUYPCIIRAF-UHFFFAOYSA-N

Formula: C30H45F4NO3

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]: 543.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.29		Crippen Method
logp	8.864		Crippen Method
mcvol	425.010	ml/mol	McGowan Method
rinpol	3413.00		NIST Webbook
rinpol	3413.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345932&Units=SI>

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

Crippen Method: https://www.cheméo.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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