L-Proline, N-(2-fluoro-6-trifluoromethylbenzoyl)-, heptadecyl ester

Inchi: InChI=1S/C30H45F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-23-38-29(37)26-21-1
Inchikey: PCESWSHAVYHNKI-UHFFFAOYSA-N
Formula: C30H45F4NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1c(F)cccc1C(F)(F)F
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	3483.00		NIST Webbook
rinpol	3483.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345908&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.