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

Inchi: InChI=1S/C28H41F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-36-27(35)24-19-16-20-3
InchiKey: IBIWXJXSJAFVPO-UHFFFAOYSA-N
Formula: C28H41F4NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1F
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	3243.00		NIST Webbook
rinpol	3243.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346002&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

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