L-Proline, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C28H42F3NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-36-28(34)23-17-16-18-
InchiKey: LMTUFNLXXNROMG-UHFFFAOYSA-N
Formula: C28H42F3NO4
SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 513.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.13		Crippen Method
logp	7.352		Crippen Method
mcvol	400.930	ml/mol	McGowan Method
rinpol	3440.00		NIST Webbook
rinpol	3440.00		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=U346031&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.