L-Proline, N-(2,3,4-trifluorobenzoyl)-, undecyl ester

Inchi: InChI=1S/C23H32F3NO3/c1-2-3-4-5-6-7-8-9-10-16-30-23(29)19-12-11-15-27(19)22(28)1
InchiKey: WQJODWBDKCLUGG-UHFFFAOYSA-N
Formula: C23H32F3NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 427.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.34		Crippen Method
logp	5.783		Crippen Method
mcvol	324.610	ml/mol	McGowan Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		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=U346328&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

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