L-Proline, N-(2-trifluoromethylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C24H34F3NO3/c1-2-3-4-5-6-7-8-9-12-18-31-23(30)21-16-13-17-28(21)22(29)1
InchiKey: LOOWOWQQZZEYSU-UHFFFAOYSA-N
Formula: C24H34F3NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1C(F)(F)F
Mol. weight [g/mol]: 441.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.45		Crippen Method
logp	6.384		Crippen Method
mcvol	338.700	ml/mol	McGowan Method
rinpol	2847.00		NIST Webbook
rinpol	2847.00		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=U346212&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

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