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

Inchi: InChI=1S/C23H32F3NO3/c1-2-3-4-5-6-7-8-11-17-30-22(29)20-15-12-16-27(20)21(28)18-

InchiKey: FXQPADZRYZPKCG-UHFFFAOYSA-N

Formula: C23H32F3NO3

SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 427.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	5.994		Crippen Method
mcvol	324.610	ml/mol	McGowan Method
rinpol	2744.00		NIST Webbook
rinpol	2744.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346211&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.