L-Proline, N-(3-trifluoromethylbenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C29H44F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-22-36-28(35)26-20-17-2

InchiKey: CUMAEURPGJPTIM-UHFFFAOYSA-N

Formula: C29H44F3NO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 511.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.54		Crippen Method
logp	8.335		Crippen Method
mcvol	409.150	ml/mol	McGowan Method
rinpol	3366.00		NIST Webbook
rinpol	3366.00		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=U346352&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.