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

Inchi: InChI=1S/C25H36F3NO3/c1-2-3-4-5-6-7-8-9-10-13-19-32-24(31)22-17-14-18-29(22)23(3

InchiKey: BPLTZFGHWGPPNS-UHFFFAOYSA-N

Formula: C25H36F3NO3

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

Mol. weight [g/mol]: 455.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.87		Crippen Method
logp	6.774		Crippen Method
mcvol	352.790	ml/mol	McGowan Method
rinpol	2958.00		NIST Webbook
rinpol	2958.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346213&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.