L-Proline, N-(2,5-ditrifluoromethylbenzoyl)-, octyl ester

Other names: L-Proline, N-(2,5-ditrifluoromethylbenzoyl)-, octadecyl ester
Inchi: InChI=1S/C32H47F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-42-30(41)28-1
InchiKey: XEYRHMXADJUNTL-UHFFFAOYSA-N
Formula: C32H47F6NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 607.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.48		Crippen Method
logp	10.133		Crippen Method
mcvol	456.730	ml/mol	McGowan Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345989&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices