

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

Inchi: InChI=1S/C31H45F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-22-41-29(40)27-18-1
InchiKey: IBPRMQAEBZJBNK-UHFFFAOYSA-N
Formula: C31H45F6NO3
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 593.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.06		Crippen Method
logp	9.743		Crippen Method
mcvol	442.640	ml/mol	McGowan Method
rinpol	3266.00		NIST Webbook
rinpol	3266.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345988&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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