

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

Inchi: InChI=1S/C29H41F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-39-27(38)25-16-15-19-3
InchiKey: DDJKJCOSVYJZEV-UHFFFAOYSA-N
Formula: C29H41F6NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 565.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.23		Crippen Method
logp	8.963		Crippen Method
mcvol	414.460	ml/mol	McGowan Method
rinpol	3056.00		NIST Webbook
rinpol	3056.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U345986&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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