

L-Proline, N-(2,3,4-trifluorobenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C26H38F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-33-26(32)22-15-14-18-30(2)
InchiKey: GVMJGZTZG XKUMF-UHFFFAOYSA-N
Formula: C₂₆H₃₈F₃NO₃
SMILES: CCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 469.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.60		Crippen Method
logp	6.953		Crippen Method
mcvol	366.880	ml/mol	McGowan Method
rinpol	3147.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U346330&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

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