

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

Inchi: InChI=1S/C24H31F6NO3/c1-2-3-4-5-6-7-8-9-15-34-22(33)20-11-10-14-31(20)21(32)18-1
InchiKey: SXVBCFILNMUHQX-UHFFFAOYSA-N
Formula: C24H31F6NO3
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 495.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.13		Crippen Method
logp	7.013		Crippen Method
mcvol	344.010	ml/mol	McGowan Method
rinpol	2544.00		NIST Webbook
rinpol	2544.00		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=U345982&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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