

L-Proline, N-(3-trifluoromethylbenzoyl)-, decyl ester

Inchi: InChI=1S/C23H32F3NO3/c1-2-3-4-5-6-7-8-9-16-30-22(29)20-14-11-15-27(20)21(28)18-1
InchiKey: HGICPXUUFYWPRB-UHFFFAOYSA-N
Formula: C23H32F3NO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 427.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.03		Crippen Method
logp	5.994		Crippen Method
mcvol	324.610	ml/mol	McGowan Method
rinpol	2724.00		NIST Webbook
rinpol	2724.00		NIST Webbook

Sources

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=U346347&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/117-730-1/L-Proline-N-3-trifluoromethylbenzoyl-decyl-ester.pdf>

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