

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

Inchi:	InChI=1S/C22H30F3NO3/c1-2-3-4-5-6-7-8-15-29-21(28)19-13-10-14-26(19)20(27)17-11
InchiKey:	VPSNCVZCDJZTFT-UHFFFAOYSA-N
Formula:	C22H30F3NO3
SMILES:	CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	413.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.61		Crippen Method
logp	5.604		Crippen Method
mcvol	310.520	ml/mol	McGowan Method
rinpol	2626.00		NIST Webbook
rinpol	2626.00		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=U346346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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