

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

Inchi:	InChI=1S/C21H28F3NO3/c1-2-3-4-5-6-7-14-28-20(27)18-12-9-13-25(18)19(26)16-10-8-1
InchiKey:	GPYCYFHBOULFGH-UHFFFAOYSA-N
Formula:	C21H28F3NO3
SMILES:	CCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	399.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.19		Crippen Method
logp	5.214		Crippen Method
mcvol	296.430	ml/mol	McGowan Method
rinpol	2523.00		NIST Webbook
rinpol	2523.00		NIST Webbook

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=U346345&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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