

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

Other names:	L-Proline, N-(2,5-ditrifluoromethylbenzoyl)-, octadecyl ester
Inchi:	InChI=1S/C32H47F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-42-30(41)28-1
InchiKey:	XEYRHMxADJUNTL-UHFFFAOYSA-N
Formula:	C32H47F6NO3
SMILES:	CCCCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]:	607.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.48		Crippen Method
logp	10.133		Crippen Method
mcvol	456.730	ml/mol	McGowan Method
rinpol	3381.00		NIST Webbook
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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=U345989&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

Latest version available from:

<https://www.chemeo.com/cid/121-712-6/L-Proline-N-2-5-ditrifluoromethylbenzoyl-octyl-ester.pdf>

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