

L-Proline, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, nonyl

Inchi:
ester

InChI=1S/C22H30F3NO4/c1-3-4-5-6-7-8-9-13-30-22(28)17-11-10-12-26(17)21(27)15-14

InchiKey:

NIRYNFPSMLNPGY-UHFFFAOYSA-N

Formula:

C22H30F3NO4

SMILES:

CCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]:

429.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.62		Crippen Method
logp	5.011		Crippen Method
mcvol	316.390	ml/mol	McGowan Method
rinpol	2799.00		NIST Webbook
rinpol	2799.00		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=U346026&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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