

L-Proline, N-(3-fluoro-4-trifluoromethylbenzoyl)-, nonyl

Inchi:
ester

InChI=1S/C22H29F4NO3/c1-2-3-4-5-6-7-8-14-30-21(29)19-10-9-13-27(19)20(28)16-11-1

InchiKey:

LGOGHFSXTSRKID-UHFFFAOYSA-N

Formula:

C22H29F4NO3

SMILES:

CCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]:

431.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.94		Crippen Method
logp	5.743		Crippen Method
mcvol	312.290	ml/mol	McGowan Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U345968&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

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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