

L-Proline, N-(5-fluoro-2-trifluoromethylbenzoyl)-, hexyl

Inchi:
ester

InChI=1S/C19H23F4NO3/c1-2-3-4-5-11-27-18(26)16-7-6-10-24(16)17(25)14-12-13(20)8

InchiKey:

XPZIGPMNDYPMAF-UHFFFAOYSA-N

Formula:

C19H23F4NO3

SMILES:

CCCCCOC(=O)C1CCCN1C(=O)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]:

389.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Crippen Method
logp	4.573		Crippen Method
mcvol	270.020	ml/mol	McGowan Method
rinpol	2248.00		NIST Webbook
rinpol	2248.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U346008&Units=SI>

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>

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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