

L-Proline, N-(2-fluoro-3-trifluoromethylbenzoyl)-, butyl

Inchi:
ester

InChI=1S/C17H19F4NO3/c1-2-3-10-25-16(24)13-8-5-9-22(13)15(23)11-6-4-7-12(14(11)1

InchiKey:

SGWWGDQQGBMQYTM-UHFFFAOYSA-N

Formula:

C17H19F4NO3

SMILES:

CCCCOC(=O)C1CCCN1C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]:

361.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.85		Crippen Method
logp	3.792		Crippen Method
mcvol	241.840	ml/mol	McGowan Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=U345992&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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