

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

Inchi:
ester

InChI=1S/C15H15F4NO3/c1-2-23-14(22)12-4-3-7-20(12)13(21)10-8-9(15(17,18)19)5-6-1

InchiKey:

XAFOMHJOAVJZJQ-UHFFFAOYSA-N

Formula:

C15H15F4NO3

SMILES:

CCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]:

333.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	3.012		Crippen Method
mcvol	213.660	ml/mol	McGowan Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		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=U345917&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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