

Isonipectic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, ethyl

Inchi:
ester

InChI=1S/C16H17F4NO3/c1-2-24-15(23)10-5-7-21(8-6-10)14(22)12-9-11(17)3-4-13(12)1

InchiKey:

IOYQJIKMAOOIJT-UHFFFAOYSA-N

Formula:

C16H17F4NO3

SMILES:

CCOC(=O)C1CCN(C(=O)c2cc(F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]:

347.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.260		Crippen Method
mcvol	227.750	ml/mol	McGowan Method
rinpole	2082.00		NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361327&Units=SI>

Crippen Method:

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

Crippen Method:

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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