Isonipecotinoylisonipecotic acid, N'-(3-fluoro-6-trifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C22H26F4N2O4/c1-2-32-21(31)15-7-11-27(12-8-15)19(29)14-5-9-28(10-6-14)2

InchiKey: BPLIABPRHVQYBX-UHFFFAOYSA-N

Formula: C22H26F4N2O4

SMILES: CCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cc(F)ccc3C(F)(F)F)CC2)CC1

Mol. weight [g/mol]: 458.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	3.498		Crippen Method
mcvol	312.980	ml/mol	McGowan Method
rinpol	3232.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U361344&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