

Isonipecotinoylisonipecotic acid, N'-(2-fluoro-3-trifluoromethylbenzoyl)-, ethyl ester

Inchi:
ester

InChI=1S/C22H26F4N2O4/c1-2-32-21(31)15-8-12-27(13-9-15)19(29)14-6-10-28(11-7-14

InchiKey:

QPXIWBWESDHGIW-UHFFFAOYSA-N

Formula:

C22H26F4N2O4

SMILES:

CCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cccc(C(F)(F)F)c3F)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
rinpole	3281.00		NIST Webbook

Sources

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=U361323&Units=SI>

Crippen Method:

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

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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