

Isonipecotic acid, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, ethyl

Inchi:
ester

InChI=1S/C16H18F3NO4/c1-3-24-16(22)9-4-6-20(7-5-9)15(21)10-8-11(17)13(19)14(23-2

InchiKey:

GTBUBNSQPBFQSA-UHFFFAOYSA-N

Formula:

C16H18F3NO4

SMILES:

CCOC(=O)C1CCN(C(=O)c2cc(F)c(F)c(OC)c2F)CC1

Mol. weight [g/mol]:

345.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.76		Crippen Method
logp	2.528		Crippen Method
mcvol	231.850	ml/mol	McGowan Method
rinpola	2326.00		NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361347&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
rinpola:	Non-polar retention indices

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