

# Isonipecotic acid, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, pentyl ester

Inchi:  
InchiKey:

InChI=1S/C19H24F3NO4/c1-3-4-5-10-27-19(25)12-6-8-23(9-7-12)18(24)13-11-14(20)16

HGFVJDXQMHNOFJ-UHFFFAOYSA-N

Formula:

C19H24F3NO4

SMILES:

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

Mol. weight [g/mol]:

387.39

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	3.698		Crippen Method
mcvol	274.120	ml/mol	McGowan Method
rinpola	2630.00		NIST Webbook

## Sources

Crippen Method:

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

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U361351&Units=SI>

## 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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