

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

Inchi:  
ester

InChI=1S/C21H28F3NO4/c1-3-4-5-6-7-12-29-21(27)14-8-10-25(11-9-14)20(26)15-13-16

InchiKey:

CEICBHNBXHMDPX-UHFFFAOYSA-N

Formula:

C21H28F3NO4

SMILES:

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

Mol. weight [g/mol]:

415.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.85		Crippen Method
logp	4.478		Crippen Method
mcvol	302.300	ml/mol	McGowan Method
rinpol	2828.00		NIST Webbook
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## Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361354&Units=SI>

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>

## Legend

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

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