

# Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, octyl

Inchi:  
ester

InChI=1S/C22H29F4NO3/c1-2-3-4-5-6-7-12-30-21(29)16-8-10-27(11-9-16)20(28)17-13-1

InchiKey:

REDVKERHGUIOQT-UHFFFAOYSA-N

Formula:

C22H29F4NO3

SMILES:

CCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]:

431.46

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.59		Crippen Method
logp	5.600		Crippen Method
mcvol	312.290	ml/mol	McGowan Method
rinpole	2635.00		NIST Webbook

## Sources

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=U361452&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

## 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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