

# Isonipecotic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, nonyl

**Inchi:**  
**ester**

InChI=1S/C23H31F4NO3/c1-2-3-4-5-6-7-8-15-31-22(30)17-11-13-28(14-12-17)21(29)19

**InchiKey:**

BSXIKXFZCQVGPE-UHFFFAOYSA-N

**Formula:**

C23H31F4NO3

**SMILES:**

CCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2C(F)(F)F)CC1

**Mol. weight [g/mol]:**

445.49

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	5.991		Crippen Method
mcvol	326.380	ml/mol	McGowan Method
rinpole	2786.00		NIST Webbook

## Sources

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361336&Units=SI>

**Crippen Method:**

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

**Crippen Method:**

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

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

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