

# Isonipecotic acid, N-(3-trifluoromethylbenzoyl)-, nonyl ester

**Inchi:** InChI=1S/C23H32F3NO3/c1-2-3-4-5-6-7-8-16-30-22(29)18-12-14-27(15-13-18)21(28)19  
**InchiKey:** MXJPMAUHCCGIHZ-UHFFFAOYSA-N  
**Formula:** C23H32F3NO3  
**SMILES:** CCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1  
**Mol. weight [g/mol]:** 427.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	5.851		Crippen Method
mcvol	324.610	ml/mol	McGowan Method
rinpole	2835.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361547&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**rinpole:** Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/44-705-0/Isonipecotic-acid-N-3-trifluoromethylbenzoyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-26 09:27:20.375792498 +0000 UTC m=+16412889.296369814.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.