

# Isonipecotic acid, N-(2-trifluoromethylbenzoyl)-, heptyl ester

**Inchi:** InChI=1S/C21H28F3NO3/c1-2-3-4-5-8-15-28-20(27)16-11-13-25(14-12-16)19(26)17-9-6  
**InchiKey:** APMWSDFUGVVPS-UHFFFAOYSA-N  
**Formula:** C<sub>21</sub>H<sub>28</sub>F<sub>3</sub>NO<sub>3</sub>  
**SMILES:** CCCCCCOC(=O)C1CCN(C(=O)c2ccccc2C(F)(F)F)CC1  
**Mol. weight [g/mol]:** 399.45

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.84		Crippen Method
logp	5.071		Crippen Method
mcvol	296.430	ml/mol	McGowan Method
rinpol	2679.00		NIST Webbook
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## 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=U361492&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  
**rinpol:** Non-polar retention indices

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