

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

**Inchi:** InChI=1S/C20H26F3NO3/c1-14(2)5-4-12-27-19(26)15-8-10-24(11-9-15)18(25)16-6-3-7-1  
**InchiKey:** DUYNGVVWHOUCDY-UHFFFAOYSA-N  
**Formula:** C<sub>20</sub>H<sub>26</sub>F<sub>3</sub>NO<sub>3</sub>  
**SMILES:** CC(C)CCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1  
**Mol. weight [g/mol]:** 385.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.537		Crippen Method
mcvol	282.340	ml/mol	McGowan Method
rinpol	2499.00		NIST Webbook
rinpol	2499.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=U361545&Units=SI>

## 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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