

# Isonipecotic acid, N-(2-fluoro-5-trifluoromethylbenzoyl)-, isohexyl ester

InChI: InChI=1S/C20H25F4NO3/c1-13(2)4-3-11-28-19(27)14-7-9-25(10-8-14)18(26)16-12-15(20)  
InChIKey: RWWFXANBPLCCRO-UHFFFAOYSA-N

Formula: C<sub>20</sub>H<sub>25</sub>F<sub>4</sub>NO<sub>3</sub>  
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)CC1  
Mol. weight [g/mol]: 403.41

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Crippen Method
logp	4.676		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpole	2447.00		NIST Webbook

## Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
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=U361390&Units=SI>

## 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/16-741-1/Isonipecotic-acid-N-2-fluoro-5-trifluoromethylbenzoyl-iso-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-20 03:00:20.614056537 +0000 UTC m=+15871269.534633852.

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