

# Isonipecotinoylisonipecotic acid, N'-(4-fluoro-2-trifluoromethylbenzoyl)-, isobutyl ester

InChI: InChI=1S/C24H30F4N2O4/c1-15(2)14-34-23(33)17-7-11-29(12-8-17)21(31)16-5-9-30(10)  
InChIKey: BICSXTWHCBQDLY-UHFFFAOYSA-N

Formula: C<sub>24</sub>H<sub>30</sub>F<sub>4</sub>N<sub>2</sub>O<sub>4</sub>

SMILES: CC(C)COC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(F)cc3C(F)(F)F)CC2)CC1

Mol. weight [g/mol]: 486.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	4.135		Crippen Method
mcvol	341.160	ml/mol	McGowan Method
rinpola	3396.00		NIST Webbook

## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361261&Units=SI>

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>

## Legend

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

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