

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

InChI: InChI=1S/C18H21F4NO3/c1-11(2)10-26-17(25)12-5-7-23(8-6-12)16(24)14-4-3-13(19)9-1  
InChIKey: KCTHANMBLKDCKT-UHFFFAOYSA-N

Formula: C18H21F4NO3  
SMILES: CC(C)COC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)CC1  
Mol. weight [g/mol]: 375.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	3.896		Crippen Method
mcvol	255.930	ml/mol	McGowan Method
rinpol	2246.00		NIST Webbook
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## Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361242&Units=SI>  
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>

## 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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