

# Isonipecotinoylisonipecotic acid, N'-(2-fluoro-5-trifluoromethylbenzoyl)-, butyl ester

Inchi:  
ester

InChI=1S/C24H30F4N2O4/c1-2-3-14-34-23(33)17-8-12-29(13-9-17)21(31)16-6-10-30(11)

InchiKey: LJZCFNOQZGXAIU-UHFFFAOYSA-N

Formula: C24H30F4N2O4

SMILES: CCCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3cc(C(F)(F)F)ccc3F)CC2)CC1

Mol. weight [g/mol]: 486.50

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.42		Crippen Method
logp	4.279		Crippen Method
mcvol	341.160	ml/mol	McGowan Method
rinpol	3436.00		NIST Webbook
rinpol	3436.00		NIST Webbook

## 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=U361407&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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