

# Isonipectic acid, N-(4-fluoro-2-trifluoromethylbenzoyl)-, ethyl

**Inchi:**  
**ester**

InChI=1S/C16H17F4NO3/c1-2-24-15(23)10-5-7-21(8-6-10)14(22)12-4-3-11(17)9-13(12)1

**InchiKey:**

XXXNLZDBCRBIFZ-UHFFFAOYSA-N

**Formula:**

C16H17F4NO3

**SMILES:**

CCOC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)CC1

**Mol. weight [g/mol]:**

347.30

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.260		Crippen Method
mcvol	227.750	ml/mol	McGowan Method
rinpola	2083.00		NIST Webbook

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361240&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

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

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