

# Isonipectic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, heptyl

**Inchi:**  
**ester**

InChI=1S/C21H27F4NO3/c1-2-3-4-5-6-13-29-20(28)15-9-11-26(12-10-15)19(27)17-14-1

**InchiKey:**

KCRDRTYMPFEVMP-UHFFFAOYSA-N

**Formula:**

C21H27F4NO3

**SMILES:**

CCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2C(F)(F)F)CC1

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

417.44

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.17		Crippen Method
logp	5.210		Crippen Method
mcvol	298.200	ml/mol	McGowan Method
rinpola	2592.00		NIST Webbook

## Sources

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361334&Units=SI>

**Crippen Method:**

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

**Crippen Method:**

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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

Latest version available from:

<https://www.cheméo.com/cid/25-543-1/Isonipectic-acid-N-3-fluoro-6-trifluoromethylbenzoyl-heptyl-ester.pdf>

Generated by Cheméo on 2024-04-29 22:48:07.283086772 +0000 UTC m=+16720136.203664083.

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