

# Isonipectic acid, N-(2-fluoro-6-trifluoromethylbenzoyl)-, propyl ester

InChI: InChI=1S/C17H19F4NO3/c1-2-10-25-16(24)11-6-8-22(9-7-11)15(23)14-12(17(19,20)21)13  
InChIKey: CBWPLBHBGZQPPX-UHFFFAOYSA-N  
Formula: C17H19F4NO3  
SMILES: CCCOC(=O)C1CCN(C(=O)c2c(F)cccc2C(F)(F)F)CC1  
Mol. weight [g/mol]: 361.33

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.50		Crippen Method
logp	3.650		Crippen Method
mcvol	241.840	ml/mol	McGowan Method
rinpol	2224.00		NIST Webbook

## Sources

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>  
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361284&Units=SI>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/26-518-8/Isonipectic-acid-N-2-fluoro-6-trifluoromethylbenzoyl-propyl-ester.pdf>

Generated by Cheméo on 2024-04-19 20:32:50.816623678 +0000 UTC m=+15848019.737200990.

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