Isonipecotic 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)4

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/ci990307l

Crippen Method: 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