Isonipecotic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, heptyl ester

Inchi: 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
rinpol	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.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices