Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, pentadecyl ester

Inchi: InChI=1S/C29H43F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-19-37-28(36)23-15-17-34(1

InchiKey: STAXFUJHEIYZTA-UHFFFAOYSA-N

Formula: C29H43F4NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]: 529.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.52		Crippen Method
logp	8.331		Crippen Method
mcvol	410.920	ml/mol	McGowan Method
rinpol	3344.00		NIST Webbook

Sources

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=U361459&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices