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

Inchi: InChI=1S/C29H44F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-22-36-28(35)24-18-20-33(2

InchiKey: INVCKMRXPAHYMC-UHFFFAOYSA-N

Formula: C29H44F3NO3

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]: 511.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.19		Crippen Method
logp	8.192		Crippen Method
mcvol	409.150	ml/mol	McGowan Method
rinpol	3479.00		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=U361553&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