Isonipecotic acid, N-(2-trifluoromethylbenzoyl)-, dodecyl ester

Inchi: InChI=1S/C26H38F3NO3/c1-2-3-4-5-6-7-8-9-10-13-20-33-25(32)21-16-18-30(19-17-21)2

InchiKey: KYAQKXSWEWDNAJ-UHFFFAOYSA-N

Formula: C26H38F3NO3

SMILES: CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2C(F)(F)F)CC1

Mol. weight [g/mol]: 469.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.93		Crippen Method
logp	7.022		Crippen Method
mcvol	366.880	ml/mol	McGowan Method
rinpol	3213.00		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=U361497&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