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

Inchi: InChI=1S/C24H34F3NO3/c1-2-3-4-5-6-7-8-9-17-31-23(30)19-13-15-28(16-14-19)22(29)2

InchiKey: ZEOWJAFYJHCRMZ-UHFFFAOYSA-N

Formula: C24H34F3NO3

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

Mol. weight [g/mol]: 441.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	6.242		Crippen Method
mcvol	338.700	ml/mol	McGowan Method
rinpol	2950.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361548&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

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