

Isonipecotic acid, N-(3-fluoro-4-trifluoromethylbenzoyl)-, tridecyl ester

InChI: InChI=1S/C27H39F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-19-35-26(34)21-15-17-32(18-16-20)33
InChIKey: RBUTWGVWLCXGRM-UHFFFAOYSA-N

Formula: C27H39F4NO3

SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(F)c2)CC1

Mol. weight [g/mol]: 501.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.68		Crippen Method
logp	7.551		Crippen Method
mcvol	382.740	ml/mol	McGowan Method
rinpol	3249.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361477&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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