

Isonipecotic acid, N-(4-fluoro-2-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)33-27-25-24-23-22-21
InChIKey: RNPZUKGCMHCOIU-UHFFFAOYSA-N

Formula: C27H39F4NO3

SMILES: CCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)cc2C(F)(F)F)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	3215.00		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=U361253&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

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