

Isonipecotic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, undecyl ester

InChI: InChI=1S/C25H35F4NO3/c1-2-3-4-5-6-7-8-9-10-15-33-24(32)19-11-13-30(14-12-19)23(31)16-20-21-22-25
InChIKey: PCZQXDDQQLYSEG-UHFFFAOYSA-N

Formula: C25H35F4NO3

SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1

Mol. weight [g/mol]: 473.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.85		Crippen Method
logp	6.771		Crippen Method
mcvol	354.560	ml/mol	McGowan Method
rinpol	2944.00		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=U361455&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

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