

Isonipecotic acid, N-(3-fluorobenzoyl)-, undecyl ester

Inchi:	InChI=1S/C24H36FNO3/c1-2-3-4-5-6-7-8-9-10-18-29-24(28)20-14-16-26(17-15-20)23(27)
InchiKey:	AQHIGQNRZQEESC-UHFFFAOYSA-N
Formula:	C24H36FNO3
SMILES:	CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1
Mol. weight [g/mol]:	405.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.74		Crippen Method
logp	5.752		Crippen Method
mcvol	335.160	ml/mol	McGowan Method
rinpola	3163.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361527&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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