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

Inchi: InChI=1S/C25H38FNO3/c1-2-3-4-5-6-7-8-9-10-11-19-30-25(29)21-15-17-27(18-16-21)24
InchiKey: NYMAHWVAUQFVEU-UHFFFAOYSA-N
Formula: C25H38FNO3
SMILES: CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1
Mol. weight [g/mol]: 419.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.16		Crippen Method
logp	6.142		Crippen Method
mcvol	349.250	ml/mol	McGowan Method
rinpol	3267.00		NIST Webbook
rinpol	3267.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361528&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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