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

Inchi: InChI=1S/C25H39NO4/c1-3-4-5-6-7-8-9-10-11-19-30-25(28)21-15-17-26(18-16-21)24(27

InchiKey: SMISCKNWQLDRLF-UHFFFAOYSA-N

Formula: C25H39NO4

SMILES: CCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(OC)c2)CC1

Mol. weight [g/mol]: 417.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.53		Crippen Method
logp	5.621		Crippen Method
mcvol	353.350	ml/mol	McGowan Method
rinpol	3447.00		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=U361183&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