Isonipecotic acid, N-benzoyl-, undecyl ester

Inchi: InChI=1S/C24H37NO3/c1-2-3-4-5-6-7-8-9-13-20-28-24(27)22-16-18-25(19-17-22)23(26)
InchiKey: IUJMBWBRYKILMG-UHFFFAOYSA-N
Formula: C24H37NO3
SMILES: CCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccccc2)CC1
Mol. weight [g/mol]: 387.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	5.613		Crippen Method
mcvol	333.390	ml/mol	McGowan Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		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=U360981&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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