Isonipecotic acid, N-(2-methoxybenzoyl)-, pentyl ester

Inchi: InChI=1S/C19H27NO4/c1-3-4-7-14-24-19(22)15-10-12-20(13-11-15)18(21)16-8-5-6-9-17

InchiKey: MHECOSDQLJKSFI-UHFFFAOYSA-N

Formula: C19H27NO4

SMILES: CCCCCOC(=O)C1CCN(C(=O)c2ccccc2OC)CC1

Mol. weight [g/mol]: 333.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	3.281		Crippen Method
mcvol	268.810	ml/mol	McGowan Method
rinpol	2696.00		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=U361188&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