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

Inchi: InChI=1S/C21H31NO4/c1-3-4-5-6-9-16-26-21(24)17-12-14-22(15-13-17)20(23)18-10-7-8

InchiKey: JOPBNFMBFFDAPF-UHFFFAOYSA-N

Formula: C21H31NO4

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

Mol. weight [g/mol]: 361.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.86		Crippen Method
logp	4.061		Crippen Method
mcvol	296.990	ml/mol	McGowan Method
rinpol	2911.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361191&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