Isonipecotic acid, N-(4-methylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C20H29NO3/c1-3-4-5-6-15-24-20(23)18-11-13-21(14-12-18)19(22)17-9-7-16(2

InchiKey: ZQYPTFRPVVCQOB-UHFFFAOYSA-N

Formula: C20H29NO3

SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2ccc(C)cc2)CC1

Mol. weight [g/mol]: 331.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.79		Crippen Method
logp	3.971		Crippen Method
mcvol	277.030	ml/mol	McGowan Method
rinpol	2785.00		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=U361118&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