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

Inchi: InChI=1S/C22H33NO3/c1-3-4-5-6-7-8-17-26-22(25)20-13-15-23(16-14-20)21(24)19-11-9

InchiKey: OHTKSIKIEVQELA-UHFFFAOYSA-N

Formula: C22H33NO3

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

Mol. weight [g/mol]: 359.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	4.751		Crippen Method
mcvol	305.210	ml/mol	McGowan Method
rinpol	3016.00		NIST Webbook
rinpol	3016.00		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=U361120&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.