Isonipecotic acid, N-(3-methylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C21H31NO3/c1-3-4-5-6-7-15-25-21(24)18-11-13-22(14-12-18)20(23)19-10-8-9

InchiKey: VOUQHUMMMUERDX-UHFFFAOYSA-N

Formula: C21H31NO3

SMILES: CCCCCCCOC(=O)C1CCN(C(=O)c2cccc(C)c2)CC1

Mol. weight [g/mol]: 345.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.361		Crippen Method
mcvol	291.120	ml/mol	McGowan Method
rinpol	2866.00		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=U361102&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