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

Inchi: InChI=1S/C18H25NO3/c1-13(2)12-22-18(21)15-7-9-19(10-8-15)17(20)16-6-4-5-14(3)11-

InchiKey: XNNAXSQISJLQTB-UHFFFAOYSA-N

Formula: C18H25NO3

SMILES: Cc1cccc(C(=O)N2CCC(C(=O)OCC(C)C)CC2)c1

Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.71		Crippen Method
logp	3.046		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2503.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361097&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

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