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

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

InchiKey: HIZAGOIXKJAHKQ-UHFFFAOYSA-N

Formula: C18H25NO3

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

Mol. weight [g/mol]: 303.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.96		Crippen Method
logp	3.191		Crippen Method
mcvol	248.850	ml/mol	McGowan Method
rinpol	2552.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361098&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

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