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

Inchi: InChI=1S/C16H21NO3/c1-3-20-16(19)13-7-9-17(10-8-13)15(18)14-6-4-5-12(2)11-14/h4-

InchiKey: BZBCAUBBMRPKMF-UHFFFAOYSA-N

Formula: C16H21NO3

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

Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	2.410		Crippen Method
mcvol	220.670	ml/mol	McGowan Method
rinpol	2336.00		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=U361095&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