

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/h4-6,11-13,15-17,19-20/t16
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

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