

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

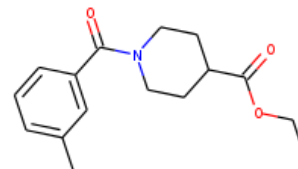
InChI: InChI=1S/C16H21NO3/c1-3-20-16(19)13-7-9-17(10-8-13)15(18)14-6-4-5-12(2)11-14/h4-6,11,13H,3,7-10H2,1-2H3

InChI Key: BZBCAUBBMRPKMF-UHFFFAOYSA-N

Formula: C16H21NO3

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

Molecular Weight: 275.34



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	2.41		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/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/h4-6,11,13H,3,7-10H2,1-2H3](http://webbook.nist.gov/cgi/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/h4-6,11,13H,3,7-10H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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