

4-Methylvaleric acid, picolinyl ester

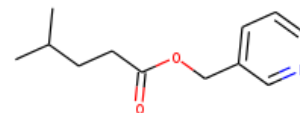
InChI: InChI=1S/C12H17NO2/c1-10(2)5-6-12(14)15-9-11-4-3-7-13-8-11/h
3-4,7-8,10H,5-6,9H2,1-2H3

InChI Key: BTZVIEPPMAHNOJ-UHFFFAOYSA-N

Formula: C₁₂H₁₇NO₂

SMILES: CC(C)CCC(=O)OCc1ccnc1

Molecular Weight: 207.27



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	2.56		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H17NO2/c1-10\(2\)5-6-12\(14\)15-9-11-4-3-7-13-8-11/h3-4,7-8,10H,5-6,9H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H17NO2/c1-10(2)5-6-12(14)15-9-11-4-3-7-13-8-11/h3-4,7-8,10H,5-6,9H2,1-2H3)

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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