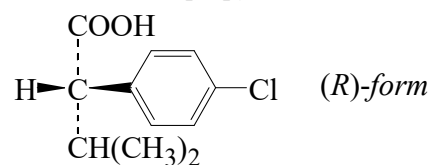




>>Entry Name: 2-(4-Chlorophenyl)-3-methylbutanoic acid

Synonym(s): 4-Chloro- α -(1-methylethyl)benzeneacetic acid, 9Cl. 4-Chloro- α -isopropylbenzeneacetic acid



CAS Registry Number: 2012-74-0

Molecular Formula: C₁₁H₁₃ClO₂

Molecular Weight: 212.675

Accurate Mass: 212.060407

Percentage Composition: C 62.12%; H 6.16%; Cl 16.67%; O 15.05%

Metabolism: Metab. of Fenvalerate [DLC14-U](#) in animals

>>Variant: (R)-form

CAS Registry Number: 63640-09-5

Molecular Formula: C₁₁H₁₃ClO₂

Molecular Weight: 212.675

Accurate Mass: 212.060407

Percentage Composition: C 62.12%; H 6.16%; Cl 16.67%; O 15.05%

Optical Rotation: [α]_D²⁰ -46.9 (c, 2 in CHCl₃) (96.1% op)

>>Variant: (S)-form

CAS Registry Number: 55332-38-2

Molecular Formula: C₁₁H₁₃ClO₂

Molecular Weight: 212.675

Accurate Mass: 212.060407

Percentage Composition: C 62.12%; H 6.16%; Cl 16.67%; O 15.05%

Physical Description: Cryst.

Melting Point: Mp 106-107°

Optical Rotation: [α]_D²¹ +47.5 (c, 2 in CHCl₃) (97.4% op)

>>Variant: (±)-form

CAS Registry Number: 55291-27-5

Molecular Formula: C₁₁H₁₃ClO₂

Molecular Weight: 212.675

Accurate Mass: 212.060407

Percentage Composition: C 62.12%; H 6.16%; Cl 16.67%; O 15.05%

Use/Importance: Key intermed. in the synth. of Fenvalerate [DLC14-U](#)

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 88-89°

>>Derivative: Chloride

CAS Registry Number: 51631-50-6

Extra CAS Registry Numbers(s): 66230-05-5

Molecular Formula: C₁₁H₁₂Cl₂O

Molecular Weight: 231.121

Accurate Mass: 230.026519

Percentage Composition: C 57.17%; H 5.23%; Cl 30.68%; O 6.92%

Physical Description: Oil

>>Derivative: Nitrile

Synonym(s): 1-(4-Chlorophenyl)-1-cyano-2-methylpropane

CAS Registry Number: 81951-76-0

Extra CAS Registry Numbers(s): 2012-81-9

Molecular Formula: C₁₁H₁₂ClN

Molecular Weight: 193.675

Accurate Mass: 193.065826

Percentage Composition: C 68.22%; H 6.24%; Cl 18.31%; N 7.23%

Physical Description: Oil

Boiling Point: Bp_{1.8} 93.5°

References: