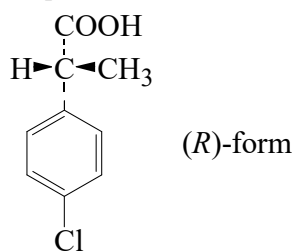




>>Entry Name: 2-(4-Chlorophenyl)propanoic acid

Synonym(s): 4-Chloro- α -methylbenzeneacetic acid, 9Cl. *p*-Chlorohydratropic acid



CAS Registry Number: 938-95-4

Related CAS Registry Numbers(s): 73037-67-9

Molecular Formula: C₉H₉ClO₂

Molecular Weight: 184.622

Accurate Mass: 184.029107

Percentage Composition: C 58.55%; H 4.91%; Cl 19.20%; O 17.33%

>>Variant: (*R*)-form

CAS Registry Number: 105879-62-7

Molecular Formula: C₉H₉ClO₂

Molecular Weight: 184.622

Accurate Mass: 184.029107

Percentage Composition: C 58.55%; H 4.91%; Cl 19.20%; O 17.33%

>>Derivative: Me ester

CAS Registry Number: 86010-00-6

Molecular Formula: C₁₀H₁₁ClO₂

Molecular Weight: 198.648

Accurate Mass: 198.044757

Percentage Composition: C 60.46%; H 5.58%; Cl 17.85%; O 16.11%

Physical Description: Liq.

Optical Rotation: [α]_D -67 (c, 1.1 in CHCl₃)

>>Variant: (*S*)-form

CAS Registry Number: 105879-63-8

Molecular Formula: C₉H₉ClO₂

Molecular Weight: 184.622

Accurate Mass: 184.029107

Percentage Composition: C 58.55%; H 4.91%; Cl 19.20%; O 17.33%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 78-78.5°

Optical Rotation: [α]_D²⁰ +124 (c, 1.25 in AcOH). [α]_D²⁰ +112 (c, 1.4 in EtOH)

>>Derivative: Me ester

CAS Registry Number: 137044-27-0

Molecular Formula: C₁₀H₁₁ClO₂

Molecular Weight: 198.648

Accurate Mass: 198.044757

Percentage Composition: C 60.46%; H 5.58%; Cl 17.85%; O 16.11%

Physical Description: Liq.

Boiling Point: Bp_{0.5} 82°

Refractive Index: n_D²⁰ 1.5155

>>Derivative: Amide

Molecular Formula: C₉H₁₀ClNO

Molecular Weight: 183.637

Accurate Mass: 183.045091

Percentage Composition: C 58.87%; H 5.49%; Cl 19.31%; N 7.63%; O 8.71%

Physical Description: Needles (H₂O)

Melting Point: Mp 119.5°