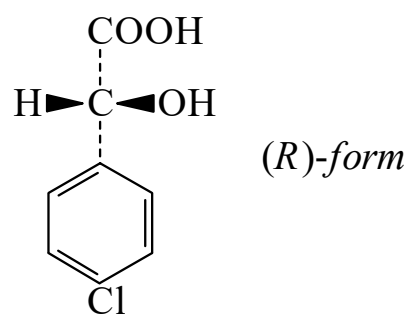




>>Entry Name: 2-(4-Chlorophenyl)-2-hydroxyacetic acid

Synonym(s): 4-Chloro- α -hydroxybenzeneacetic acid, 9Cl. *p*-Chloromandelic acid, 8Cl. *p*-Chlorophenylglycollic acid



CAS Registry Number: 492-86-4

Molecular Formula: $C_8H_7ClO_3$

Molecular Weight: 186.594

Accurate Mass: 186.008372

Percentage Composition: C 51.50%; H 3.78%; Cl 19.00%; O 25.72%

Fluka: 24990

Rare Chemicals Library: S44477-4

>>Variant: (*R*)-form

CAS Registry Number: 32189-36-9

Molecular Formula: $C_8H_7ClO_3$

Molecular Weight: 186.594

Accurate Mass: 186.008372

Percentage Composition: C 51.50%; H 3.78%; Cl 19.00%; O 25.72%

Physical Description: Cryst. (C_6H_6 or $CHCl_3$)

Melting Point: Mp 121°

Optical Rotation: $[\alpha]_D^{25} -136$ (c, 0.7 in Me_2CO)

>>Variant: ($\pm$)-form

CAS Registry Number: 7138-34-3

Molecular Formula: $C_8H_7ClO_3$

Molecular Weight: 186.594

Accurate Mass: 186.008372

Percentage Composition: C 51.50%; H 3.78%; Cl 19.00%; O 25.72%

Use/Importance: Used as a 1mM aq. soln. for photometric detn. of Zr (λ_{max} 266 nm), Mo(*VI*) (λ_{max} 630 nm, ϵ 106000, $CHCl_3$)

Physical Description: Cryst. ($CHCl_3$ /petrol)

Melting Point: Mp 119-120°

Solubility: Sol. H_2O

pKa Value: pK_{a1} 3.15 (25°)

>>Derivative: Me ether

CAS Registry Number: 4674-24-2

Molecular Formula: $C_9H_9ClO_3$

Molecular Weight: 200.621

Accurate Mass: 200.024022

Percentage Composition: C 53.88%; H 4.52%; Cl 17.67%; O 23.92%

Physical Description: Cryst. (C_6H_6 /petrol)

Melting Point: Mp 85-88°

>>Derivative: Amide

Molecular Formula: $C_8H_8ClNO_2$

Molecular Weight: 185.609

Accurate Mass: 185.024356

Percentage Composition: C 51.77%; H 4.34%; Cl 19.10%; N 7.55%; O 17.24%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 122-123°