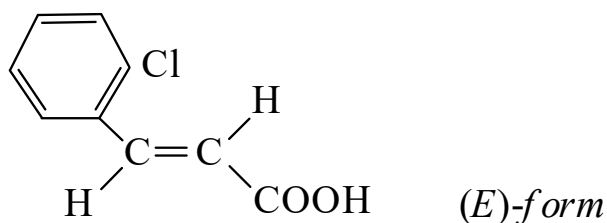




>>Entry Name: 3-(2-Chlorophenyl)-2-propenoic acid

Synonym(s): *o*-Chlorocinnamic acid



CAS Registry Number: 3752-25-8

Molecular Formula: C₉H₇ClO₂

Molecular Weight: 182.606

Accurate Mass: 182.013457

Percentage Composition: C 59.20%; H 3.86%; Cl 19.41%; O 17.52%

Hazard & Toxicity: LD₅₀ (mus, orl) 989 mg/kg

Aldrich: C3139-2

>>Variant: (*E*)-form

CAS Registry Number: 939-58-2

Molecular Formula: C₉H₇ClO₂

Molecular Weight: 182.606

Accurate Mass: 182.013457

Percentage Composition: C 59.20%; H 3.86%; Cl 19.41%; O 17.52%

Physical Description: Yellow cryst. (EtOH)

Melting Point: Mp 212°

pKa Value: pK_{a1} 4.23 (25°)

>>Derivative: Me ester

CAS Registry Number: 42174-97-0

Molecular Formula: C₁₀H₉ClO₂

Molecular Weight: 196.633

Accurate Mass: 196.029107

Percentage Composition: C 61.08%; H 4.61%; Cl 18.03%; O 16.27%

Physical Description: Cryst. (petrol)

Melting Point: Mp 10.5°

Boiling Point: Bp 278-279°

>>Derivative: Amide

CAS Registry Number: 15851-90-8

Molecular Formula: C₉H₈ClNO

Molecular Weight: 181.621

Accurate Mass: 181.029441

Percentage Composition: C 59.52%; H 4.44%; Cl 19.52%; N 7.71%; O 8.81%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 168°

>>Variant: (*Z*)-form

CAS Registry Number: 704-96-1

Molecular Formula: C₉H₇ClO₂

Molecular Weight: 182.606

Accurate Mass: 182.013457

Percentage Composition: C 59.20%; H 3.86%; Cl 19.41%; O 17.52%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 136-137°

>>Derivative: Amide

Physical Description: Cryst. (EtOH)

Melting Point: Mp 112°

References: