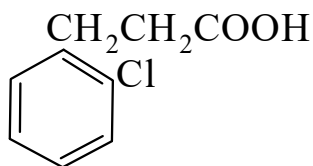




>>Entry Name: 3-(2-Chlorophenyl)propanoic acid

Synonym(s): 2-Chlorobenzenepropanoic acid, 9Cl. *o*-Chlorohydrocinnamic acid, 8Cl. 3-*o*-Chlorophenylpropionic acid



CAS Registry Number: 1643-28-3

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: Needles or leaflets (H₂O, EtOH or C₆H₆/petrol)

Melting Point: Mp 102° (94.5-95.5°, 96-99°)

pKa Value: pK_a 4.58

Rare Chemicals Library: S38021-0

>>Derivative: Me ester

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 255°

>>Derivative: Chloride

CAS Registry Number: 52085-97-9

Molecular Formula: C₉H₈Cl₂O

Molecular Weight: 203.067

Accurate Mass: 201.995219

Percentage Composition: C 53.23%; H 3.97%; Cl 34.92%; O 7.88%

Physical Description: Liq.

Boiling Point: Bp₂₆ 147.5-149°

>>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 (C₆H₆)

Melting Point: Mp 119°

>>Derivative: Nitrile

CAS Registry Number: 7315-17-5

Molecular Formula: C₉H₈ClN

Molecular Weight: 165.622

Accurate Mass: 165.034526

Percentage Composition: C 65.27%; H 4.87%; Cl 21.41%; N 8.46%

Physical Description: Liq.

Boiling Point: Bp 267-268°

Aldrich: 34663-2

Rare Chemicals Library: S50066-6

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1482C, (*nmr*)

Fieser, L.F. *et al.*, *J.A.C.S.*, 1937, **59**, 394, (*synth*)

Grebenyuk, A.D. *et al.*, *Zh. Obshch. Khim.*, 1955, **25**, 269; *CA*, **50**, 1639, (*synth*)

Tóth, G. *et al.*, *Synth. Commun.*, 1995, **25**, 3067, (*synth*)