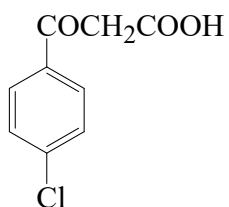




>>Entry Name: 3-(4-Chlorophenyl)-3-oxopropanoic acid

Synonym(s): 4-Chloro-β-oxobenzenepropanoic acid, 9Cl. *p*-Chlorobenzoylacetic acid, 8Cl



CAS Registry Number: 17589-68-3

Molecular Formula: C₉H₇ClO₃

Molecular Weight: 198.605

Accurate Mass: 198.008372

Percentage Composition: C 54.43%; H 3.55%; Cl 17.85%; O 24.17%

Physical Description: Cryst. (Et₂O/petrol)

Melting Point: Mp 121-122° (dec.). Mp 232° (prob. incorr.)

>>Derivative: Me ester

CAS Registry Number: 22027-53-8

Molecular Formula: C₁₀H₉ClO₃

Molecular Weight: 212.632

Accurate Mass: 212.024022

Percentage Composition: C 56.49%; H 4.27%; Cl 16.67%; O 22.57%

Physical Description: Cryst.

Melting Point: Mp 36-37°

Boiling Point: Bp₁₂ 172°

>>Derivative: Et ester

CAS Registry Number: 2881-63-2

Molecular Formula: C₁₁H₁₁ClO₃

Molecular Weight: 226.659

Accurate Mass: 226.039672

Percentage Composition: C 58.29%; H 4.89%; Cl 15.64%; O 21.18%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 37-38°

Boiling Point: Bp₁₈ 181-182°

>>Derivative: Nitrile

Synonym(s): 4'-Chloro-2-cyanoacetophenone. 1-Chloro-4-(cyanoacetyl)benzene

CAS Registry Number: 4640-66-8

Molecular Formula: C₉H₆ClNO

Molecular Weight: 179.605

Accurate Mass: 179.013791

Percentage Composition: C 60.19%; H 3.37%; Cl 19.74%; N 7.80%; O 8.91%

Physical Description: Cryst. (C₆H₆/petrol)

Melting Point: Mp 129-130°

References:

Thorp, L. *et al.*, *J.A.C.S.*, 1915, **37**, 1258-1264, (*synth*)

Long, R.S., *J.A.C.S.*, 1947, **69**, 990-995, (*nitrile*)

Straub, T.S. *et al.*, *J.A.C.S.*, 1972, **94**, 8881-8888, (*synth, props*)

Lee, L.F. *et al.*, *J. Het. Chem.*, 1985, **22**, 1621-1630, (*Et ester, synth, pmr*)

Org. Synth., Coll. Vol., 7, 1990, 213-215, (*Et ester*)