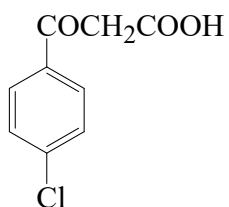




>>Entry Name: **3-(4-Chlorophenyl)-3-oxopropanoic acid**

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



**CAS Registry Number:** 17589-68-3

**Molecular Formula:** C<sub>9</sub>H<sub>7</sub>ClO<sub>3</sub>

**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. (Et<sub>2</sub>O/petrol)

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

>>Derivative: Me ester

**CAS Registry Number:** 22027-53-8

**Molecular Formula:** C<sub>10</sub>H<sub>9</sub>ClO<sub>3</sub>

**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:** Bp<sub>12</sub> 172°

>>Derivative: Et ester

**CAS Registry Number:** 2881-63-2

**Molecular Formula:** C<sub>11</sub>H<sub>11</sub>ClO<sub>3</sub>

**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:** Bp<sub>18</sub> 181-182°

>>Derivative: Nitrile

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

**CAS Registry Number:** 4640-66-8

**Molecular Formula:** C<sub>9</sub>H<sub>6</sub>ClNO

**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. (C<sub>6</sub>H<sub>6</sub>/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*)