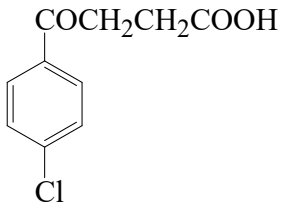
>>**Entry Name: 4-(4-Chlorophenyl)-4-oxobutanoic acid**

Synonym(s): 4-Chloro-γ-oxobenzenebutanoic acid, ^{9Cl}, ^{8Cl}. 3-(4-Chlorobenzoyl)propanoic acid



CAS Registry Number: 3984-34-7
Related CAS Registry Numbers(s): 64081-77-2 64350-81-8

Molecular Formula: $C_{10}H_9ClO_3$
Molecular Weight: 212.632
Accurate Mass: 212.024022
Percentage Composition: C 56.49%; H 4.27%; Cl 16.67%; O 22.57%
General Statement: Shows tautomerism to hydroxylactone form
Use/Importance: Intermed. for azepines
Physical Description: Cryst. (MeOH aq.)
Melting Point: Mp 131°
pKa Value: pK_a 5.7 (25°,50% EtOH aq.)

>>**Derivative:** *S*-Benzylthiouronium salt

Physical Description: Cryst. (EtOH)
Melting Point: Mp 159-160°

>>**Derivative:** Me ester

CAS Registry Number: 7148-01-8
Molecular Formula: $C_{11}H_{11}ClO_3$
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. (Et_2O)
Melting Point: Mp 63°

>>**Derivative:** Et ester

CAS Registry Number: 53503-49-4
Molecular Formula: $C_{12}H_{13}ClO_3$
Molecular Weight: 240.686
Accurate Mass: 240.055322
Percentage Composition: C 59.88%; H 5.44%; Cl 14.73%; O 19.94%
Physical Description: Cryst.
Melting Point: Mp 58°

>>**Derivative:** Benzyl ester

Molecular Formula: $C_{17}H_{15}ClO_3$
Molecular Weight: 302.756
Accurate Mass: 302.070972
Percentage Composition: C 67.44%; H 4.99%; Cl 11.71%; O 15.85%
Physical Description: Liq.
Boiling Point: Bp_4 251-253°

References:

Allen, C.F.H. *et al.*, *Can. J. Res.*, 1934, **II**, 382-390, *(synth, Me ester)*
Fr. Pat., 1974, 2 203 625; *CA*, **81**, 120608y, *(Et ester)*
Aeberli, P. *et al.*, *J. Med. Chem.*, 1976, **19**, 436-438, *(synth)*
Fadnavis, N.W.*, Indian J. Chem., Sect. B*, 1979, **17**, 518-519, *(synth, Et ester)*