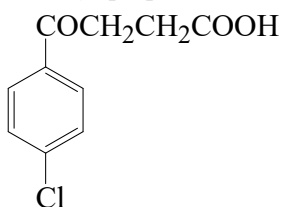




>>Entry Name: 4-(4-Chlorophenyl)-4-oxobutanoic acid

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: C₁₀H₉ClO₃

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: 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. (Et₂O)

Melting Point: Mp 63°

>>Derivative: Et ester

CAS Registry Number: 53503-49-4

Molecular Formula: C₁₂H₁₃ClO₃

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: C₁₇H₁₅ClO₃

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: Bp₄ 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*)