



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

Synonym(s): 4-Chlorobenzenepropanoic acid, 9Cl. *p*-Chlorohydrocinnamic acid, 8Cl. 3-*p*-Chlorophenylpropionic acid

CAS Registry Number: 2019-34-3

Structure by analogy with 3-(2-Chlorophenyl)propanoic acid, [DXD04-C](#)

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%

Melting Point: Mp 126° (121-122.5°)

pKa Value: pK_a 4.61

>>Derivative: Et ester

CAS Registry Number: 7116-36-1

Molecular Formula: C₁₁H₁₃ClO₂

Molecular Weight: 212.675

Accurate Mass: 212.060407

Percentage Composition: C 62.12%; H 6.16%; Cl 16.67%; O 15.05%

Physical Description: Liq.

Boiling Point: Bp₁₅ 158-159°

>>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: Leaflets (C₆H₆)

Melting Point: Mp 133°

>>Derivative: Nitrile

Physical Description: Liq.

Boiling Point: Bp₁₅ 153-156°

References:

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Nesmeyanov, A.N. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1955, 933; *CA*, **50**, 11279, (*synth*)

Fuchs, R. *et al.*, *J.O.C.*, 1962, **27**, 733, (*synth*)

Wittstruck, T.A. *et al.*, *J.A.C.S.*, 1967, **89**, 3803, (*pmr*)

Kadentsev, V.I. *et al.*, *Izv. Akad. Nauk SSSR, Ser. Khim.*, 1972, 2440; *CA*, **78**, 96726, (*ms*)

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