



>>Entry Name: 3-Chlorophenylacetic acid, 8Cl

Synonym(s): 3-Chlorobenzeneacetic acid, 9Cl. *m*-Chloro- α -toluic acid

CAS Registry Number: 1878-65-5

Structure by analogy with 2-Chlorophenylacetic acid, [DWZ58-U](#)

Molecular Formula: C₈H₇ClO₂

Molecular Weight: 170.595

Accurate Mass: 170.013457

Percentage Composition: C 56.33%; H 4.14%; Cl 20.78%; O 18.76%

Physical Description: Cryst. (H₂O or EtOH)

Melting Point: Mp 77° (74.5°)

pKa Value: pK_{a1} 4.11 (25°)

Aldrich: C6335-9

Fluka: 25930

>>Derivative: Me ester

CAS Registry Number: 53088-68-9

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%

Boiling Point: Bp₉ 120-121°

Refractive Index: n_D²⁰ 1.5238

>>Derivative: Et ester

CAS Registry Number: 14062-29-4

Molecular Formula: C₁₀H₁₁ClO₂

Molecular Weight: 198.648

Accurate Mass: 198.044757

Percentage Composition: C 60.46%; H 5.58%; Cl 17.85%; O 16.11%

Boiling Point: Bp₂₆ 146-148°

Refractive Index: n_D^{24.2} 1.5100

>>Derivative: Chloride

CAS Registry Number: 41904-39-6

Molecular Formula: C₈H₆Cl₂O

Molecular Weight: 189.04

Accurate Mass: 187.979569

Percentage Composition: C 50.83%; H 3.20%; Cl 37.51%; O 8.46%

Physical Description: Burgundy liq.

>>Derivative: Nitrile

Synonym(s): 3-Chlorobenzeneacetonitrile, 9Cl. *m*-Chlorobenzyl cyanide

CAS Registry Number: 1529-41-5

Molecular Formula: C₈H₆ClN

Molecular Weight: 151.595

Accurate Mass: 151.018876

Percentage Composition: C 63.38%; H 3.99%; Cl 23.39%; N 9.24%

Boiling Point: Bp₁₀ 135°

Hazard & Toxicity: LD₅₀ (mus, ipr) 38 mg/kg

Aldrich: C2780-8

Fluka: 23860

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 1007C; 1490C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 154A; 432B, (*ir*)

Kenner, J. *et al.*, *J.C.S.*, 1934, 679, (*synth*)

Campbell, N. *et al.*, *J.C.S.*, 1948, 1251, (*synth*)

Heathcock, C.H. *et al.*, *J.O.C.*, 1990, **55**, 798, (*chloride, synth, pmr, cmr*)