



>>Entry Name: 4-Chlorophenylacetic acid, 8Cl

Synonym(s): 4-Chlorobenzeneacetic acid, 9Cl. *p*-Chloro- α -toluic acid

CAS Registry Number: 1878-66-6

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 petrol)

Melting Point: Mp 106°

pKa Value: pK_{a1} 4.18 (25°)

Hazard & Toxicity: LD₅₀ (mus, ipr) 1350 mg/kg

Aldrich: 13926-2

Fluka: 25931

Sigma: C5262

>>Derivative: Me ester

CAS Registry Number: 52449-43-1

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: Bp₆ 114-115°

Rare Chemicals Library: S73457-8

>>Derivative: Et ester

CAS Registry Number: 14062-24-9

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: Bp₁₃ 130°

Rare Chemicals Library: S66874-5

>>Derivative: Chloride

CAS Registry Number: 25026-34-0

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%

Boiling Point: Bp₁₅ 127-129°

Aldrich: 46250-0

>>Derivative: Nitrile

Synonym(s): 4-Chlorobenzeneacetonitrile, 9Cl. *p*-Chlorobenzyl cyanide

CAS Registry Number: 140-53-4

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%

Physical Description: Needles (petrol)

Melting Point: Mp 31-32°

Boiling Point: Bp 264-267°. Bp₁₂ 137-139°

Aldrich: C2800-6

Fluka: 23880

References: