



>>Entry Name: 3-Chloro-4-methylbenzoic acid, 9Cl

Synonym(s): 3-Chloro-*p*-toluic acid

CAS Registry Number: 5162-82-3

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: Leaflets

Melting Point: Mp 200-202° (194-196°)

pKa Value: pK_a 4.06 (20°, 1% EtOH)

>>Derivative: Me ester

CAS Registry Number: 56525-63-4

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 28°

Boiling Point: Bp_{6.5} 105-107°

>>Derivative: Et ester

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: Bp₁₄ 135°

>>Derivative: Nitrile

Synonym(s): 3-Chloro-4-methylbenzonitrile. 2-Chloro-4-cyano-1-methylbenzene. 2-Chloro-4-cyanotoluene

CAS Registry Number: 21423-81-4

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%

Melting Point: Mp 48-49°

Aldrich: 14970-5

References:

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