



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

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

CAS Registry Number: 5162-82-3

Molecular Formula: C<sub>8</sub>H<sub>7</sub>ClO<sub>2</sub>

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<sub>a</sub> 4.06 (20°, 1% EtOH)

>>Derivative: Me ester

CAS Registry Number: 56525-63-4

Molecular Formula: C<sub>9</sub>H<sub>9</sub>ClO<sub>2</sub>

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<sub>6.5</sub> 105-107°

>>Derivative: Et ester

Molecular Formula: C<sub>10</sub>H<sub>11</sub>ClO<sub>2</sub>

Molecular Weight: 198.648

Accurate Mass: 198.044757

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

Boiling Point: Bp<sub>14</sub> 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: C<sub>8</sub>H<sub>6</sub>ClN

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:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1529C, (*nmr*)

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Hintikka, S.V., *CA*, 1925, **19**, 42, (*synth*)

Stempel, G.H. *et al.*, *J.A.C.S.*, 1951, **73**, 455, (*synth*)

Peltier, D. *et al.*, *Bull. Soc. Chim. Fr.*, 1960, 1141

Crandall, E.W. *et al.*, *J.O.C.*, 1967, **32**, 134, (*synth*, *uv*)

Otto, J. *et al.*, *Pol. J. Chem. (Rocz. Chem.)*, 1972, **46**, 1551; *CA*, **78**, 57909t, (*synth*)