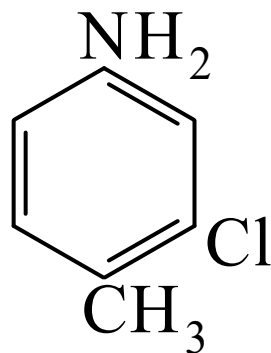




>>Entry Name: 3-Chloro-4-methylaniline

Synonym(s): 3-Chloro-4-methylbenzenamine, 9Cl. 3-Chloro-*p*-toluidine. 4-Amino-2-chlorotoluene



CAS Registry Number: 95-74-9

Molecular Formula: C₇H₈ClN

Molecular Weight: 141.6

Accurate Mass: 141.034526

Percentage Composition: C 59.38%; H 5.69%; Cl 25.04%; N 9.89%

Melting Point: Mp 26°

Boiling Point: Bp 237-238.5°. Bp₁₂ 113-114°

pKa Value: pK_{a1} 4.05 (25°)

Hazard & Toxicity: Fl. p. 117°. LD₅₀ (rat, orl) 1500 mg/kg

Aldrich: 23632-2

Supelco: 44-2384

>>Derivative: *N*-Ac

Synonym(s): *N*-(3-Chloro-4-methylphenyl)acetamide, 9Cl. 3-Chloro-4-methylacetanilide. 4-Acetamido-2-chlorotoluene

CAS Registry Number: 7149-79-3

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%

Use/Importance: Used as 2% soln. in C₆H₆ for extraction photometric detn. of W (with SCN⁽⁻⁾; λ_{max} 405 nm, ε 9200)

Physical Description: Cryst. (EtOH or hexane)

Melting Point: Mp 85° (from EtOH). Mp 104-105° (from hexane)

Solubility: Sol. C₆H₆

Rare Chemicals Library: S75308-4

>>Derivative: *N*-Benzoyl

CAS Registry Number: 10286-78-9

Molecular Formula: C₁₄H₁₂ClNO

Molecular Weight: 245.708

Accurate Mass: 245.060741

Percentage Composition: C 68.44%; H 4.92%; Cl 14.43%; N 5.70%; O 6.51%

Physical Description: Needles

Melting Point: Mp 122°

Rare Chemicals Library: S60429-1

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