



>>Entry Name: 4-Chloro-3-nitroaniline, 8Cl

Synonym(s): 4-Chloro-3-nitrobenzenamine, 9Cl

CAS Registry Number: 635-22-3

Molecular Formula: C₆H₅ClN₂O₂

Molecular Weight: 172.57

Accurate Mass: 172.003955

Percentage Composition: C 41.76%; H 2.92%; Cl 20.54%; N 16.23%; O 18.54%

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 103°

pKa Value: pK_{a1} 1.93 (25°)

Hazard & Toxicity: Eye and skin irritant. Skin absorption may cause dermatitis, methaemoglobinaemia leading to cyanosis, liver and kidney damage. Symptoms of exposure may be delayed. LD₅₀ (rat, orl) 400 mg/kg. Exp. reprod. effects

Aldrich: C5821-5

Fluka: 25390

>>Derivative: N-Ac

CAS Registry Number: 5540-60-3

Molecular Formula: C₈H₇ClN₂O₃

Molecular Weight: 214.608

Accurate Mass: 214.01452

Percentage Composition: C 44.77%; H 3.29%; Cl 16.52%; N 13.05%; O 22.37%

Melting Point: Mp 150°

>>Derivative: N,N-Di-Me

CAS Registry Number: 50817-44-2

Molecular Formula: C₈H₉ClN₂O₂

Molecular Weight: 200.624

Accurate Mass: 200.035255

Percentage Composition: C 47.89%; H 4.52%; Cl 17.67%; N 13.96%; O 15.95%

Physical Description: Yellow needles (MeOH)

Melting Point: Mp 83°

References:

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Heppollette, R.L. *et al.*, *J.A.C.S.*, 1953, **75**, 4265, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, CJA185

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