



>>Entry Name: 2-Chloro-5-nitroaniline, 8Cl
Synonym(s): 2-Chloro-5-nitrobenzenamine, 9Cl

CAS Registry Number: 6283-25-6

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 (petrol)

Melting Point: Mp 121°

pKa Value: pK_{a1} 0.64 (25°)

Hazard & Toxicity: Skin absorption may cause dermatitis, methaemoglobinaemia leading to cyanosis, liver and kidney damage. Symptoms of exposure may be delayed

Aldrich: C5815-0

Fluka: 25375

>>Derivative: N-Ac

CAS Registry Number: 4031-81-6

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 156°

>>Derivative: N-Me

Molecular Formula: C₇H₇ClN₂O₂

Molecular Weight: 186.597

Accurate Mass: 186.019605

Percentage Composition: C 45.06%; H 3.78%; Cl 19.00%; N 15.01%; O 17.15%

Melting Point: Mp 99°

>>Derivative: N,N-Di-Me

CAS Registry Number: 17815-97-3

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%

Melting Point: Mp 64-65°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1366B, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1210D, (*ir*)

Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 1169D, (*nmr*)

Blanksma, J.J., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1946, **65**, 207, (*synth*)

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