



>>Entry Name: 2-Chloro-4-nitroaniline, 8Cl

Synonym(s): 2-Chloro-4-nitrobenzenamine, 9Cl

CAS Registry Number: 121-87-9

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 108°

pKa Value: pK_{a1} -0.94 (25°)

Hazard & Toxicity: Skin absorption may cause dermatitis, methaemoglobinaemia leading to cyanosis, liver and kidney damage. Symptoms of exposure may be delayed. LD₅₀ (rat, orl) 6430 mg/kg

Aldrich: 10165-6

Fluka: 25370

Supelco: 4-8020

>>Derivative: N-Ac

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%

Physical Description: Prisms (EtOH)

Melting Point: Mp 139°

>>Derivative: N-Benzoyl

Molecular Formula: C₁₃H₉ClN₂O₃

Molecular Weight: 276.678

Accurate Mass: 276.03017

Percentage Composition: C 56.43%; H 3.28%; Cl 12.81%; N 10.12%; O 17.35%

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 161°

>>Derivative: N-Me

CAS Registry Number: 6085-92-3

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%

Physical Description: Yellow needles

Melting Point: Mp 116-117°

>>Derivative: N,N-Di-Me

CAS Registry Number: 6213-19-0

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 plates (EtOH)

Melting Point: Mp 78°

Rare Chemicals Library: S88679-3

References:

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Lutskii, A.E. *et al.*, *J. Gen. Chem. USSR (Engl. Transl.)*, 1976, **46**, 2348, (pmr)

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