



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

CAS Registry Number: 1635-61-6

Molecular Formula: $C_6H_5ClN_2O_2$
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: Golden leaflets (MeOH)
Melting Point: Mp 126.5-127°
pKa Value: $pK_{a1} -1.54$ (25°)

Aldrich: 26905-0

Fluka: 25395

Rare Chemicals Library: S66808-7

>>Derivative: *N*-Ac
Synonym(s): 5-Chloro-2-nitroacetanilide

CAS Registry Number: 5443-33-4
Molecular Formula: $C_8H_7ClN_2O_3$
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: Cryst. (EtOH)
Melting Point: Mp 117-118°
Rare Chemicals Library: S71520-4

>>Derivative: *N*-Me

CAS Registry Number: 35966-84-8
Molecular Formula: $C_7H_7ClN_2O_2$
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: Orange needles (EtOH)
Melting Point: Mp 106-107°

>>Derivative: *N,N*-Di-Me

Molecular Formula: $C_8H_9ClN_2O_2$
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 prisms (petrol)
Melting Point: Mp 49°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 745A, (*nmr*)
Fuson, R.C. *et al.*, *J.O.C.*, 1947, **12**, 799, (*synth*)
Archer, G.A. *et al.*, *J. Med. Chem.*, 1977, **20**, 1312, (*synth*)