



>>Entry Name: 3-Chloro-4-nitroaniline, 8Cl  
Synonym(s): 3-Chloro-4-nitrobenzenamine, 9Cl

CAS Registry Number: 825-41-2

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: Yellow leaflets ( $C_6H_6$ )  
Melting Point: Mp 161-162°  
pKa Value:  $pK_{a1}$  0.26 (HCl aq.)

Rare Chemicals Library: S38912-9

>>Derivative: *N*-Ac

CAS Registry Number: 712-33-4  
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: Pale-yellow needles (EtOH aq.)  
Melting Point: Mp 144.5-145°

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

CAS Registry Number: 17815-98-4  
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 needles (EtOH)  
Melting Point: Mp 125-126°

#### References:

Hodgson, H.H. *et al.*, *J.C.S.*, 1929, 2917, (*synth*)  
White, W.N. *et al.*, *J.O.C.*, 1977, **42**, 166, (*synth*)