



>>Derivative: Nitrile

Synonym(s): 2-Cyano-4-nitroaniline

CAS Registry Number: 17420-30-3

Molecular Formula: $C_7H_5N_3O_2$

Molecular Weight: 163.135

Accurate Mass: 163.038177

Percentage Composition: C 51.54%; H 3.09%; N 25.76%; O 19.61%

Use/Importance: Dyestuffs intermed.

Physical Description: Yellow needles (H_2O)

Melting Point: Mp 200-207° (209°)

Aldrich: 15349-4

Fluka: 28535

>>Derivative: N-Me

CAS Registry Number: 3484-33-1

Molecular Formula: $C_8H_8N_2O_4$

Molecular Weight: 196.162

Accurate Mass: 196.048408

Percentage Composition: C 48.98%; H 4.11%; N 14.28%; O 32.62%

Physical Description: Pale yellow leaflets (EtOH)

Melting Point: Mp 259 dec.°

References:

Aldrich Library of ^{13}C and 1H FT NMR Spectra, 1992, **2**, 1130C, (*nmr*)

Baudet, H.P., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1924, **43**, 710, (*nitrile*)

King, R.R. *et al.*, *Phytochemistry*, 1998, **49**, 1265-1267, (*isol, pmr, cmr*)