



>>Entry Name: 4-Methyl-3,5-dinitroaniline

Synonym(s): 4-Methyl-3,5-dinitrobenzenamine, 9Cl. 3,5-Dinitro-*p*-toluidine, 8Cl

CAS Registry Number: 19406-51-0

Molecular Formula: C₇H₇N₃O₄

Molecular Weight: 197.15

Accurate Mass: 197.043657

Percentage Composition: C 42.65%; H 3.58%; N 21.31%; O 32.46%

Physical Description: Yellow needles (H₂O)

Melting Point: Mp 171°

Hazard & Toxicity: LD₅₀ (rat, orl) 959 mg/kg

Rare Chemicals Library: S74931-1

Supelco: R47-4245

>>Derivative: Hydrochloride

CAS Registry Number: 70343-11-2

Physical Description: Yellow

Melting Point: Mp 171°

>>Derivative: *N*-Ac

Molecular Formula: C₉H₉N₃O₅

Molecular Weight: 239.187

Accurate Mass: 239.054222

Percentage Composition: C 45.19%; H 3.79%; N 17.57%; O 33.45%

Physical Description: Needles (EtOH)

Melting Point: Mp 223°

>>Derivative: *N*-Di-Me

Molecular Formula: C₉H₁₁N₃O₄

Molecular Weight: 225.204

Accurate Mass: 225.074957

Percentage Composition: C 48.00%; H 4.92%; N 18.66%; O 28.42%

Physical Description: Yellow needles (AcOH)

Melting Point: Mp 192°

References:

Parkes, G.D. *et al.*, *J.C.S.*, 1948, 1275, (*synth*)

Nielsen, A.T. *et al.*, *J.O.C.*, 1979, **44**, 2499, (*synth, pmr*)