



>>Entry Name: 4,5-Dimethyl-2-nitroaniline

Synonym(s): 6-Nitro-3,4-xylidine. 4,5-Dimethyl-2-nitrobenzenamine

CAS Registry Number: 6972-71-0

Structure by analogy with 2,3-Dimethyl-4-nitroaniline, [DZX27-V](#)

Molecular Formula: C₈H₁₀N₂O₂

Molecular Weight: 166.179

Accurate Mass: 166.074228

Percentage Composition: C 57.82%; H 6.07%; N 16.86%; O 19.26%

Physical Description: Brown-red prisms (EtOH)

Melting Point: Mp 139-140°

Aldrich: D17220-0

>>Derivative: N-Formyl

Molecular Formula: C₉H₁₀N₂O₃

Molecular Weight: 194.19

Accurate Mass: 194.069143

Percentage Composition: C 55.67%; H 5.19%; N 14.43%; O 24.72%

Physical Description: Yellow prisms

Melting Point: Mp 107-109°

>>Derivative: N-Ac

Molecular Formula: C₁₀H₁₂N₂O₃

Molecular Weight: 208.216

Accurate Mass: 208.084793

Percentage Composition: C 57.69%; H 5.81%; N 13.45%; O 23.05%

Physical Description: Pale yellow needles (EtOH)

Melting Point: Mp 107°

>>Derivative: N-Me

CAS Registry Number: 17978-54-0

Molecular Formula: C₉H₁₂N₂O₂

Molecular Weight: 180.206

Accurate Mass: 180.089878

Percentage Composition: C 59.99%; H 6.71%; N 15.55%; O 17.76%

Physical Description: Red powder

Melting Point: Mp 131-132°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1380A, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 771A, (*nmr*)

Diepolder, E., *Ber.*, 1909, **42**, 2917, (*synth, N-Ac*)

Suguya, T. *et al.*, *Synthesis*, 1995, 1257, (*N-formyl, synth, pmr*)

Brown, S.A. *et al.*, *Synth. Commun.*, 1996, **26**, 4065, (*N-Me*)