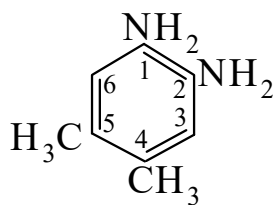




>>Entry Name: **1,2-Diamino-4,5-dimethylbenzene**

Synonym(s): 4,5-Dimethyl-1,2-benzenediamine, 9CI. 4,5-Dimethyl-*o*-phenylenediamine. 4,5-Diamino-*o*-xylene



CAS Registry Number: 3171-45-7

Molecular Formula: C₈H₁₂N₂

Molecular Weight: 136.196

Accurate Mass: 136.100048

Percentage Composition: C 70.55%; H 8.88%; N 20.57%

Biological Source: Prod. by a mutant of *Aspergillus nidulans*

Use/Importance: Reagent for the spectrophotometric detn. of 21-hydroxycorticosteroids and ascorbic acid and extraction-photometric detn. of NO₂⁽⁻⁾ ($\lambda_{\max}$ 405 nm, ϵ 1050, butanol)

Physical Description: Leaflets

Melting Point: Mp 127-129°

Solubility: Sol. H₂O

pKa Value: pK_{a1} 0.8; pK_{a2} 2.66; pK_{a3} 3.52; pK_{a4} 5.15; pK_{a5} 6.52; pK_{a6} 7.71 (25°)

Hazard & Toxicity: Irritant

Aldrich: D17660-5

Sigma: D5516

>>Derivative: 1-*N*-Formyl

CAS Registry Number: 132382-43-5

Molecular Formula: C₉H₁₂N₂O

Molecular Weight: 164.207

Accurate Mass: 164.094963

Percentage Composition: C 65.83%; H 7.37%; N 17.06%; O 9.74%

Physical Description: Prisms (MeOH)

Melting Point: Mp 169-171°

>>Derivative: 1,2-*N*-Di-Ac

Molecular Formula: C₁₂H₁₆N₂O₂

Molecular Weight: 220.271

Accurate Mass: 220.121178

Percentage Composition: C 65.43%; H 7.32%; N 12.72%; O 14.53%

Physical Description: Needles

Melting Point: Mp 227-228°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 537C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1237D, (*ir*)

Aldrich Library of IR Spectra, 2nd Ed., 651G, (*ir*)

Aldrich Library of NMR Spectra, **5**, 82A, (*pmr*)

Nölting, E. *et al.*, *Ber.*, 1901, **34**, 2251, (*synth*)

Sadique, J. *et al.*, *Curr. Sci.*, 1966, **35**, 336, (*isol*)

Braeuniger, H. *et al.*, *Pharmazie*, 1969, **24**, 24, (*synth*)

Lin, E. *et al.*, *Mikrochim. Acta*, 1970, 652, (*detn*, NO₂⁽⁻⁾)

Gorog, S. *et al.*, *Anal. Chem.*, 1972, **44**, 1079

Ceré, V. *et al.*, *Tetrahedron*, 1972, **28**, 3271, (*uv*)

Szepesi, G., *Fresenius' Z. Anal. Chem.*, 1973, **265**, 334, (*use*)

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