

N,N-bis[(1,5-dimethylpyrazol-3-yl)methyl]para-toluidine

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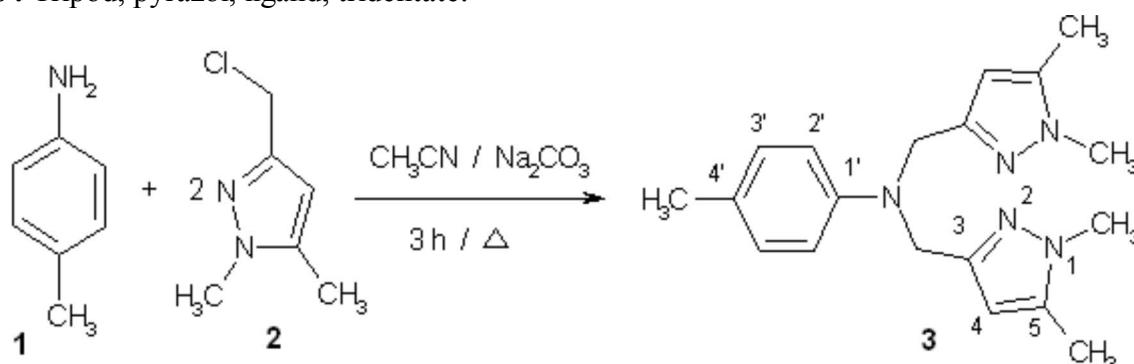
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Received: 24 October 2005 / Accepted: 15 January 2006 / Published: 1 June 2006

Keywords : Tripod, pyrazol, ligand, tridentate.



The mixture of para-toluidine **1** (0.535 g, 5 mmol), 3-chloromethyl-1,5-dimethylpyrazol **2** (1.44 g, 10 mmol) and sodium carbonate (4.24 g, 40 mmol) in acetonitrile (50 mL) was refluxed for three hours [1, 2, 3]. The solvent was removed at reduced pressure. The residue was purified through a silica column (CH₂Cl₂) to give the product **3** (726 mg, 45 % yield) as a white solid.

Melting point: 98 - 100°C (CCl₄)

IR (KBr, cm⁻¹): 3020 (v=C-H); 2960 (vC-H, CH₃); 2920 (vC-H, CH₂); 2875 (vC-H, N-CH₃); 1620 (vC=N); 1530 (vC=C); 1430; 1390 (δC-N); 1340; 1235; 1185; 940; 800 (δ=C-H); 780.

¹H-NMR (CDCl₃, 300 MHz): δ= 6.94 (d, 2 H, H_{2'}, J = 8.4 Hz); 6.78 (d, 2 H, H_{3'}, J = 8.4 Hz); 5.85 (s, 2 H, C_{4'-H}); 4.46 (s, 4 H, N-CH₂-pz); 3.69 (s, 6 H, N-CH₃); 2.19 (s, 3 H, CH₃-C₆H₄); 2.16 (s, 6 H, C₅-CH₃).

¹³C-NMR (CDCl₃, 75 MHz): δ= 149.72 (C3); 143.50 (C1'); 139.51(C5); 129.85 (C3'); 125.42 (C4'); 113.54 (C2'); 104.51(C4); 49.34 (N-CH₂-pz); 36.25 (N-CH₃); 20.62 (CH₃-C₆H₄); 11.65 (C5-CH₃).

MS (EI), m/z: 323 (5.4 %); 228 (0.4 %); 214 (100 %); 109 (24.5 %); 91 (4.4 %); 77 (0.5 %); 56 (4.9 %); 40 (3.5 %).

References and Notes:

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Sample Availability: Available from MDPI.

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