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(Z)-3-(2-Nitrophenyl)-2-(4-methylphenyl)acrylonitrile

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(2Z)-3-(2-Nitrophenyl)-2-(4-methylphenyl)acrylonitrile (3) was prepared by Knoevenagel condensation of 2-nitrobenzaldehyde 1 and 4-methylphenylacetonitrile 2 in ethanol using KOH as a base [1,2]. 2-Nitrobenzaldehyde 1 (3.01 g, 0.02 mol) and 4-methylphenylacetonitrile 2 (3.32 g, 0.02 mol) in ethanol (35 mL) were heated under reflux for seven minutes. Potassium hydroxide (1.12 g, 0.02 mol) was added in one portion and the reflux was continued for two hours. The reaction mixture was cooled to room temperature and the solid formed was filtered, washed with water and finally with ethanol (2 x 30 mL) and dried. The product was recrystallized from ethanol as yellow crystals (2.63g, 95%). M.p. 142-144 °C.

 $UV \; l_{max} \; (nm; \; EtOH)/e \; (dm^3.mol^{-1}.cm^{-1}) \; 350/15500.$

IR (cm⁻¹; KBr Disk) 2215 (CN), 1606 (C=C).

 1 H-NMR (400 MHz; CDCl₃, Me₄Si, d_H): 8.24 (1H, d, J= 9.4 Hz), 8.00 (1H, s, CH=C), 7.94 (1H, d, J = 7.7 Hz), 7.77 (1H, d), 7.64 (1H, dd), 7.60 (2H,d, 8.1 Hz), 7.28 (2H, d, 8.2 Hz), 2.38 (3H, s, MePh).

¹³C-NMR (100 MHz; CDCl₃, Me₄Si, d_C): 21.2, 108.6, 110.5, 110.8, 118.8, 124.2, 125.6, 126.8, 129.7, 131.9, 138.9, 141.1, 148.9 and 150.9.

Elemental Analysis: Calculated for C₁₆H₁₂N₂O₂ (264.26): C 72.72, H 4.58, N 10.60; Found: C 72.61, H 4.76, N 10.45.

References

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