2-(1,3-Benzodioxol-5-yl)ethylene-1,1,2-tricarbonitrile

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![Chemical Structure]

2-(1,3-benzodioxol-5-yl)ethylene-1,1,2-tricarbonitrile (2), was prepared from (1,3-benzodioxol-5-ylmethylene)malononitrile (1) and sodium cyanide, followed by oxidation using bromine [1,2]. A solution of 1 (1.0 g, 5.0 mmol) in DMF (25 mL) was cooled to 5 °C followed by dropwise addition of sodium cyanide (0.25 g, 5.0 mmol) in water (10 mL). When the addition was completed, the reaction mixture was stirred at room temperature for 3 hrs. Bromine (5 mL) was added and the stirring was continued for further two hours. 1-Hexene (50 mL) was added to destroy the excess bromine. The reaction mixture was poured into water and the precipitated solid was collected by filtration. The product was recrystallized from 1:1 toluene:chloroform as deep orange crystals (0.85 g, 75%).


UV λmax (nm; Chloroform)/ε (dm³.mol⁻¹.cm⁻¹) 344/6600, 438/11800.

IR (cm⁻¹; KBr Disk) 2226 (CN), 1609 (C=C).

¹H-NMR (400 MHz; CDCl₃; Me₄Si, δH): 6.20 (2H, s, OCH₂O), 7.02 (1H, d, J = 9.72 Hz), 7.59 (1H, s, H-2), 7.68 (1H, d, J = 8.2 Hz, H-6).

¹³C-NMR (δC): 88.24 (OCO), 103.29, 107.92, 109.64, 111.72, 111.77, 113.78, 122.97, 128.59, 140.06, 149.33, 154.73.

Elemental Analysis: Calculated for C₁₂H₅N₃O₂ (223.15): C 64.58%, H 2.24%, N 18.83%; found: C 64.36%, H 2.42%, N 18.98%.

References

