

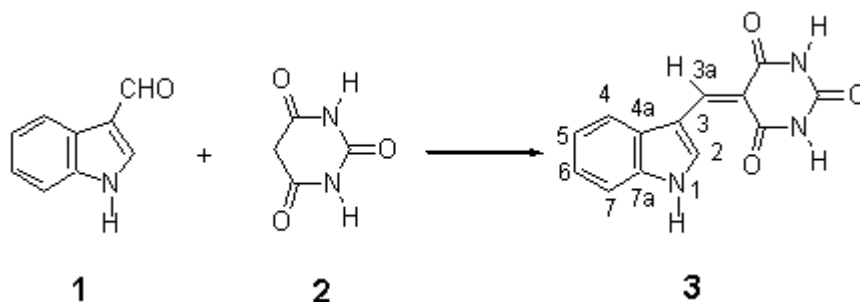
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5-(Indol-3-yl)barbituric acid

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5-(Indol-3-yl)barbituric acid **3** was prepared by knovenagel condensation of indol-3-carboxaldehyde **1** and barbituric acid **2** in ethanol using piperidine as a base [1,2]. Barbituric acid **2** (5.50 g, 0.039 mol) and indol-3-carboxaldehyde **1** (5.66 g, 0.039 mol) in ethanol (75 mL) was heated under reflux for three minutes. Piperidine (1.0 mL) was added in one portion and the reflux was continued for further five hours. The reaction mixture was cooled to room temperature and the solid formed was filtered, washed with cooled ethanol (2x20 mL) and dried. 5-(Indol-3-yle)barbituric acid **3** was recrystallized from ethanol as dark yellow powder (9.23 g, 88 %).

M.p. 250-252°C (EtOH, uncorrected).

UV (EtOH) (ϵ dm³.mol⁻¹.cm⁻¹): 220 (1910), 260 (1857), 420 (2573).

IR (cm⁻¹; KBr): 3210 (NH), 1685 (C=O), 1674 (N-CO-N), 1620 (C=C).

¹H-NMR (400 MHz, CDCl₃): 9.95 (2H, s, NH-barbituric), 8.84 (1H, s, HC=), 7.92 (1H, s, NH-indole), 7.60 (1H, d, J_{7-6} 4.1 Hz, H-7), 7.52 (1H, s, H-2), 7.40 (1H, d, J_{4-5} 4.2 Hz, H-4), 7.31 (1H, dd, J_{5-6} 3.1 Hz J_{5-4} 4.5 Hz, H-5).

¹³C-NMR (100 MHz, CDCl₃): 171.31 (N-CO-N), 164.1, 163.6 (C=O), 144.95 (C-7a), 141.5 (C-4), 140.4 (C-5), 131.5 (C-6), 123.6 (C-4a), 122.6 (C-7), 117.74 (C-2), 113.01 (C-3a).

Anal. Calc. For C₁₃H₉O₃ N₃ (255.23): C, 61.17, H, 3.55, N, 16.46; found : C, 61.22, H, 3.26; N, 16.31.

References

1. Jones, G. *Org. React.* **1967**, *15*, 203.
2. Tanaka, K.; Chen, X.; Yoneda, F. *Teteraheron* **1988**, *44*, 3241.

Sample availability: available from the authors and MDPI.

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