**5-(3,4-Dimethoxybenzylidene)-1,3-diethyl-2-thioxodihydropyrimidine-4,6(1H,5H)-dione**

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5-(3,4-Dimethoxybenzylidene)-1,3-diethyl-2-thioxodihydropyrimidine-4,6(1H,5H)-dione 3 was prepared by Knoevenagel condensation of 3,4-di-methoxybenzaldehyde 1 and N,N-diethylthiobarbituric acid 2 in ethanol using piperidine as a base [1,2].

N,N-diethylthiobarbituric acid 2 (6.0 g, 0.03 mol) and 3,4-dimethoxy- benzaldehyde 1 (5.0 g, 0.03 mol) in ethanol (50 mL) was heated under reflux for ten minutes. Piperidine (1.5 mL) was added in one portion and the reflux was continued for further three hours. The reaction mixture was cooled to room temperature and the solid formed was filtered, washed with cooled ethanol (2x 50 mL) and dried. 5-(3,4-Dimethoxybenzylidene)-1,3-diethyl-2-thioxodihydropyrimidine-4,6(1H,5H)-dione 3 was recrystallized from ethanol as deep yellow crystals (9.85 g, 94%).

M.p. 169 °C (EtOH, uncorrected).

UV λmax (nm; EtOH)/ε (dm³.mol⁻¹.cm⁻¹) 260/2009, 370/2875 and 220/2475.

IR νmax (cm⁻¹; KBr Disk) 1694 (C=O), 1670 (N-CO-N), 1632 (C=C).

¹H-NMR (400 MHz; CDCl₃; Me₄Si) dH 8.48 (1H, s, olefinic Proton), 8.35 (1H), 7.84 (1H, d, J = 8.5 Hz), 6.96 (1H, d, J= 8.5 Hz). 4.51, 4.50 (4H, t, 2xCH₂), 4.00, 3.98 (5H, s, 2xMeO), 1.33, 1.28 (6H, q, 2xCH₃).
$^{13}$C-NMR (100 MHz; CDCl$_3$; Me$_4$Si) δ C 178.8 (C=S), 161.4, 160.9 (2xC=O), 154.74, 148.16 (CH olefinic), 133.6, 131.97, 122.5, 120.8, 117.38, 109.9, 55.4, 55.02 (2x CH$_3$O), 44.1, 43.5 (2xCH$_2$), 13.0, 12.7 (2xCH$_3$).

Anal.Calc. for C$_{17}$H$_{20}$N$_2$O$_4$S (348.418): C 58.60, H 5.79, N 8.04; found : C 58.45, H 5.89, N 7.95.

References


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