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1,3-Diethyl-5-(2-methoxybenzylidene)-2-thioxodihydropyrimidine-4,6(1*H*,5*H*)-dione

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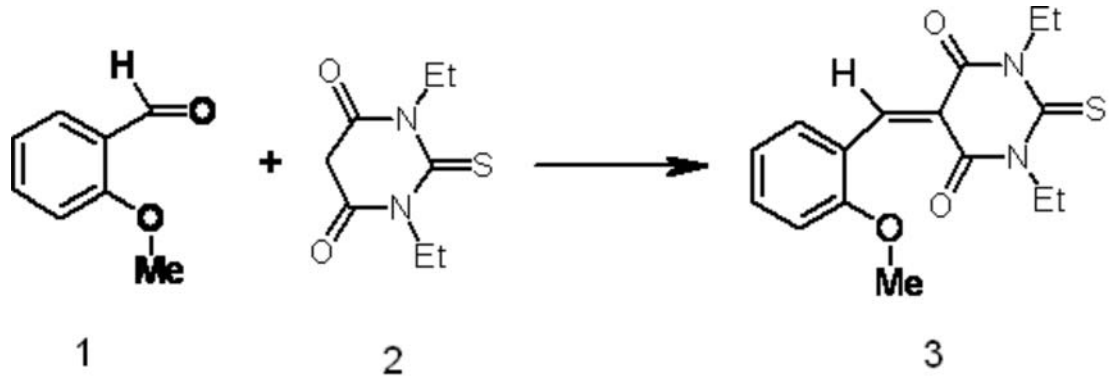

1,3-Diethyl-5-(2-methoxybenzylidene)-2-thioxodihydropyrimidine-4,6(1*H*,5*H*)-dione **3** was prepared by Knoevenagel condensation of 2-methoxybenzaldehyde **1** and N,N-diethylthiobarbituric acid **2** in ethanol using piperidine as a base [1,2].

N,N-Diethylthiobarbituric acid **2** (1.50 g, 7.5 mmol) and 2-methoxybenzaldehyde **1** (1.02 g, 0.02 mol) in ethanol (30 mL) were heated under reflux for five minutes. Piperidine (0.5 mL) 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 cold ethanol (2x 20 mL) and dried. 1,3-Diethyl-5-(2-methoxybenzylidene)-2-thioxodihydropyrimidine-4,6(1*H*,5*H*)-dione **3** was recrystallized from ethanol as deep yellow crystals (2.03 g, 85%).

M.p. 108 °C (recrystallized from EtOH, uncorrected).

UV l_{max} (nm; $CHCl_3$)/e ($dm^3.mol^{-1}.cm^{-1}$) 406/16000 and 253/ 6060.

IR nmax (KBr) cm^{-1} 2980, 1674 (C=O), 1632 (C=C), 1391 (CS).

Theoretical ($cm^{-}1$, AM1)= 1675.4, 1391.4, 1599.8

^{1}H-NMR (400 MHz; $CDCL_3$; Me_4Si) d 8.90 (1H, s, CH=C), 8.10 (1H, d, *J* = 7.84 Hz), 7.5 (1H, d, *J* = 7.24 Hz, *J* = 7.14 Hz), 7.02 (1H, t(dd), *J*= 7.6 Hz), 6.94 (1H, d, *J* = 8.42 Hz), 4.51, 4.50 (4H, t, CH_2),3.99 (3H, s, CH_3O), 1.33, 1.28 (6H, q, CH_3).

^{13}C-NMR (100 MHz, $CDCL_3$; Me_4Si) d 179 (C=S), 157.04, 155.6 (2xC=O), 148.16 (CH oliefinc), 134.4, 132.1, 122.5, 120.8, 119.2, 109.9, 43.7, 43.73 (CH_2), 13.3, 13.1 (CH_3).

Anal.Calc. for $C_{16}H_{18}N_2O_3S$ (318.392): C 60.36, H 5.70 , N 10.07; found : C 60.21, H 5.82, N 10.16.

References

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