

Short Note

5,5'-(1,4-Phenylenedimethylylidene)bis(1,3-diethyl-2-thioxodihydropyrimidine-4,6(1*H*,5*H*)-dione)

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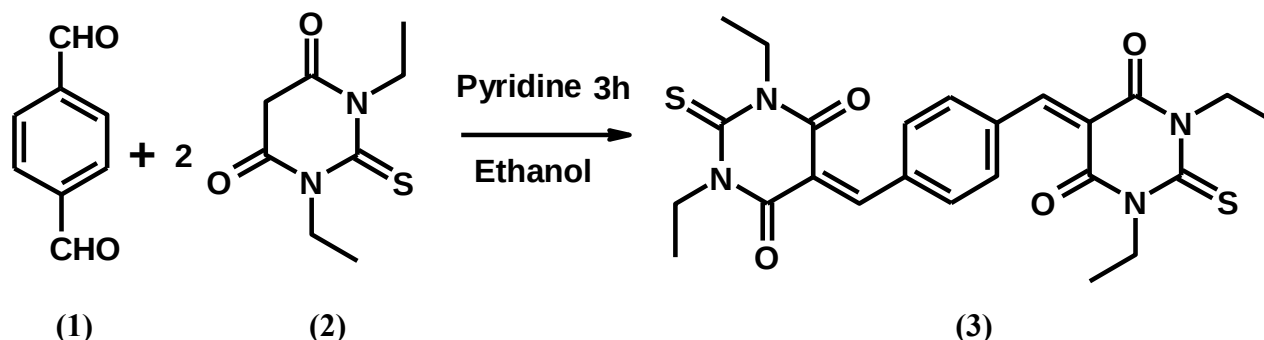
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Abstract: A novel compound, 5,5'-(1,4-phenylenedimethylylidene)bis(1,3-diethyl-2-thioxodihydropyrimidine-4,6(1*H*,5*H*)-dione) (**3**) has been synthesized by condensation of 1,3-diethyl-2-thiobarbituric acid and terephthalaldehyde in anhydrous ethanol in the presence of pyridine. The structure of this compound was established by elemental analysis, IR, ¹H-NMR, ¹³C-NMR and EI-MS spectral analysis.

Keywords: thiobarbituric acid; pyridine; Knoevenagel condensation

Barbituric acid derivatives such as phenobarbital [1] and mephobarbital [2] are used for clinical treatment of epilepsy. Thiobarbituric acid dramatically increases the diversity of biological activity. Substitution reactions at the C-5 position with different aldehydes in the presence of base or Lewis acid catalysts such as ZnCl₂ [3], CdI₂ [4], by Knoevenagel condensation give donor acceptor chromophores. These donor acceptor chromophores are applicable in optical limiting [5], electrochemical sensing [6], Langmuir film and photoinitiated polymerization [7]. As evident from the literature, it was noted that a lot of research has been carried out on donor acceptor chromophores but no work has been done on this type of bis-donor acceptor chromophore [8]. In this paper, we report the synthesis of a novel bis donor acceptor chromophore from thiobarbituric acid and terephthalaldehyde.



A mixture of 1,3-diethyl-2-thiobarbituric acid (1.49 g, 0.00746 mol) (1), terephthalaldehyde (0.5 g, 0.00373 mol) (2) and a few drops of pyridine in anhydrous ethanol (15 mL) was refluxed at 80 °C for 3 h with continuous stirring. Progress of the reaction was monitored by TLC. After completion of the reaction, the solution was cooled. The heavy precipitate thus obtained was collected by filtration and purified by recrystallization from methanol/chloroform to give the title compound (3).

Yield: 72%; m.p. 245 °C.

EI-MS m/z (rel. int.%): 499 (60) $[M+1]^+$

IR (KBr) $\nu_{\max}$ cm^{-1} : 2975 (C-H), 1606 (C=C), 1182 (C=S).

$^1\text{H-NMR}$ (CDCl_3) δ : 6.82 (s, 4H, Ar-H), 6.23 (s, 2H, C=CH), 2.65 (q, $J = 7.2$ Hz, 8H, $\text{CH}_3\text{-CH}_2\text{-N}$), 1.32 (t, $J = 7.2$ Hz, 12H, $\text{CH}_3\text{-CH}_2\text{-N}$).

$^{13}\text{C-NMR}$ (CDCl_3) δ : 173.98, 161.51, 145.35, 142.77, 126.89, 125.78, 96.31, 43.02, 42.77, 12.55, 12.08.

Anal. calc. for $\text{C}_{24}\text{H}_{26}\text{O}_4\text{N}_4\text{S}_2$: C, 57.83, H, 5.22, N, 11.24 Found: C, 57.78, H, 5.18, N, 11.22.

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