

Short Note

(2E)-1-(2,5-Dimethyl-3-thienyl)-3-(4-nitrophenyl)propenone

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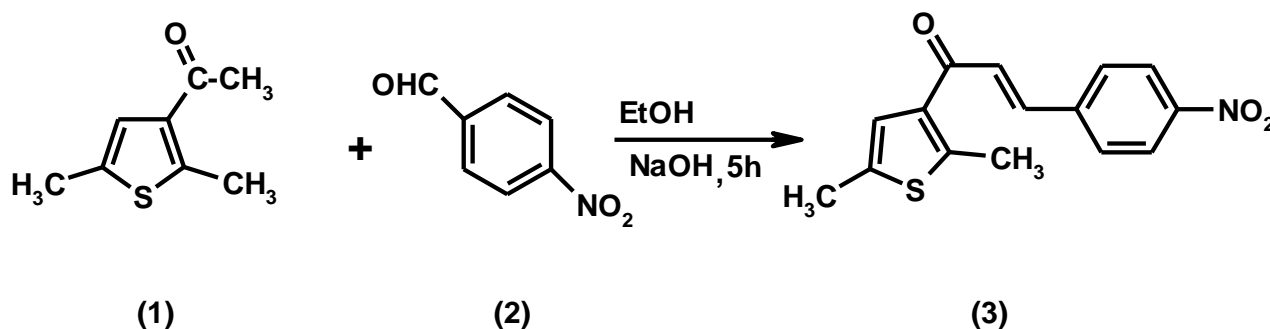
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Abstract: The title compound, (2E)-1-(2,5-dimethyl-3-thienyl)3-(4-nitrophenyl)propenone (**3**) was synthesized in high yield by reaction of 3-acetyl-2,5-dimethylthiophene and 4-nitrobenzaldehyde in the presence of sodium hydroxide. The structure of the compound was fully characterized by IR, ¹H NMR, ¹³C NMR, GC-MS spectral analysis and elemental analysis.

Keywords: chalcone; condensation; 4-nitrobenzaldehyde

1,3-Diaryl-2-propen-1-ones (chalcones) are products of condensation of simple or substituted aromatic aldehydes with simple or substituted acetophenones in the presence of alkali [1]. Chalcones constitute an important group of natural products and some of them possess a wide range of biological activities such as antimicrobial, anticancer, antitubercular, antiviral, etc. Recent studies on biological evaluation of chalcones revealed their potential to be antimalarial [2], antifungal [3], anticancer [4], antioxidant [5], tyrosinase inhibitory [6], anti-inflammatory [7] and antibacterial [8]. Some derivatives of chalcones are used as sweeteners, drugs, and sunscreen agents [9]. They are also well-known intermediates for the synthesis of various heterocyclic compounds such as pyrimidines, pyrazolines, pyrazoles, or thiazines [10]. These observations led us to synthesize a new chalcone from 3-acetyl-2,5-dimethylthiophene and 4-nitrobenzaldehyde in analogy to a previous report [11].

Scheme 1. Synthesis of the title compound (3).



A solution of 3-acetyl-2,5-dimethylthiophene (0.38 g, 0.0025 mol) and 4-nitrobenzaldehyde (0.37 g, 0.0025 mol) in an ethanolic solution of NaOH (3.0 g in 10 mL of ethanol) was stirred for 16 h at room temperature. The solution was poured into ice-cold water of pH ~2 (pH adjusted by HCl). The solid which separated was filtered and crystallized from methanol/chloroform.

Light-yellow solid; yield: 78%; m.p. 130–131 °C.

GC-MS m/z (rel. int. %): 289 (62) $[M+1]^+$.

IR (KBr) ν_{\max} cm^{-1} : 3012 (Ar-H), 2926 (C-H), 1628 (C=O), 1568 (C=C).

^1H NMR (600 MHz, $\text{DMSO-}d_6$) (δ/ppm): 8.47 (d, $J = 1.8$ Hz), 8.23 (d, $J = 1.2$ Hz), 7.73 (d, C=CH, $J = 15.6$ Hz), 7.40 (d, CH=C, $J = 15.6$ Hz), 7.89 (d, $J = 7.2$ Hz), 7.61 (d, $J = 7.8$ Hz), 7.27 (s, Ar-H), 2.72 (s, CH_3), 2.39 (s, CH_3).

^{13}C NMR (150 MHz, CDCl_3) δ : 185.23, 148.66, 148.62, 140.32, 136.79, 136.01, 135.68, 134.31, 129.98, 127.45, 125.76, 124.43, 122.16, 16.06, 15.05.

Anal. calc. for $\text{C}_{15}\text{H}_{13}\text{NO}_3\text{S}$: C, 62.70, H, 4.56, N, 4.87. Found: C, 62.66, H, 4.52, N, 4.83.

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