

Short Note

4-[[3-Cyanophenyl]imino]methyl}-3-hydroxyphenyl Tetradecanoate

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Abstract: A new Schiff base ester, 4-[[3-cyanophenyl]imino]methyl}-3-hydroxyphenyl tetradecanoate, was synthesized and its IR, ¹H NMR, ¹³C NMR and MS spectroscopic data are presented.

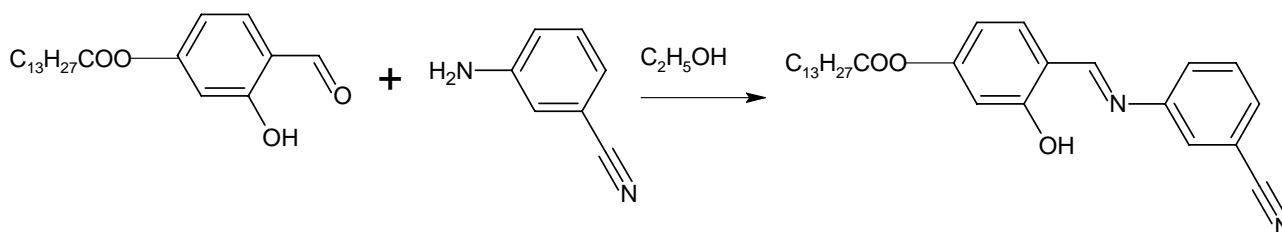
Keywords: 4-[[3-cyanophenyl]imino]methyl}-3-hydroxyphenyl tetradecanoate; Schiff base; alkyl chain

Schiff bases have received a considerable amount of attention from many researchers owing to their importance in exhibiting thermochromism and photochromism [1–4].

Synthesis

4-Formyl-3-hydroxyphenyl tetradecanoate was previously prepared via Steglich esterification [5]. In a round-bottom flask, a mixture of the 4-formyl-3-hydroxyphenyl tetradecanoate (1.74 g, 5.0 mmol), 3-aminobenzonitrile (0.59 g, 5.0 mmol) and absolute ethanol (50 mL) was refluxed with stirring for 3 hours. The reaction mixture was filtered and the solvent was removed from the filtrate by

evaporation. Recrystallization from absolute ethanol gave the title compound as a yellow solid (0.96 g, 43%).



Melting point: 85.2 °C.

MS (EI): M^+ (m/z) = 448 (4).

IR (KBr, cm^{-1}): 3439 (O-H), 2958, 2916, 2849 (C-H aliphatic); 1760 (C=O ester); 1620 (C=N); 1576, 1498 (C=C aromatic).

^1H NMR (400 MHz, CDCl_3): δ /ppm 0.88 (t, 3H, $J = 7.0$ Hz, CH_3), 1.29-1.45 {m, 20H, $\text{CH}_3(\text{CH}_2)_{10}$ -}, 1.73 (q, 2H, $J = 7.4$ Hz, $-\text{CH}_2\text{CH}_2\text{COO}-$), 2.56 (t, 2H, $J = 7.5$ Hz, $-\text{CH}_2\text{COO}-$), 6.73 (dd, 1H, $J = 2.2, 8.4$ Hz, Ar-H), 6.79 (d, 1H, $J = 2.2$ Hz, Ar-H), 7.41 (d, 1H, $J = 8.5$ Hz, Ar-H), 7.48 (dd, 1H, $J = 2.2, 7.6$ Hz, Ar-H), 7.52-7.53 (m, 1H, Ar-H), 7.54 (d, 1H, $J = 2.2$ Hz, Ar-H), 7.56 (dd, 1H, $J = 2.2, 8.5$ Hz, Ar-H), 8.61 (s, 1H, CH=N), 12.92 (s, 1H, OH).

^{13}C NMR (100 MHz, CDCl_3): δ /ppm 172.1 (COO), 164.2 (CH=N), 118.6 (C \equiv N), 162.9, 155.6, 149.7, 134.1, 130.8, 126.4, 124.9, 117.1, 114.0, 113.8, 111.0, 110.0 (aromatic carbons), 34.84 ($-\text{CH}_2\text{COO}-$), 25.26 ($-\text{CH}_2\text{CH}_2\text{COO}-$), 32.32, 30.08, 30.05, 30.00, 29.85, 29.75, 29.65, 29.47, 23.09 ($\text{CH}_3(\text{CH}_2)_{14}$ -), 14.52 (CH_3).

Elemental analysis: Calculated for $\text{C}_{28}\text{H}_{36}\text{N}_2\text{O}_3$ C, 74.97%, H, 8.09%, N, 6.24%; Found: C, 75.10%, H, 8.00%, N, 6.19%.

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