

Short Note

3-Hydroxy-4-[[(4-fluorophenyl)imino]methyl]phenyl Octadecanoate

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Abstract: A new Schiff base ester, 3-hydroxy-4-[[(4-fluorophenyl)imino]methyl]phenyl octadecanoate, was synthesized and its IR, ¹H NMR, ¹³C NMR and MS spectroscopic data are presented.

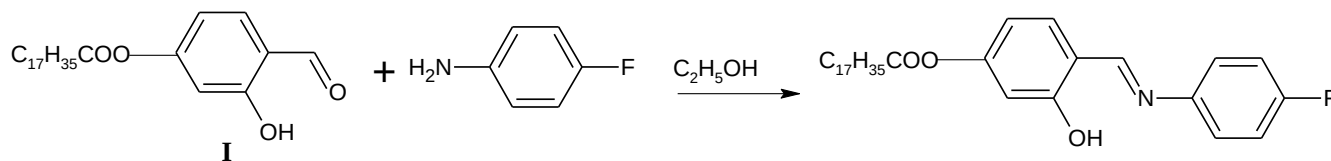
Keywords: 3-hydroxy-4-[[(4-fluorophenyl)imino]methyl]phenyl octadecanoate; Schiff base; alkyl chain

Schiff base (CH=N) compounds have received a considerable amount of attention from many researchers owing to their importance in exhibiting thermochromism and photochromism [1–3]. Aromatic Schiff bases possessing a long alkyl chain have received overwhelming attention due to their possibility to show liquid crystallinity properties such as smectic and nematic phases [4–7].

Synthesis

4-Formyl-3-hydroxyphenyl octadecanoate was previously prepared via Steglich esterification [8]. In a round-bottom flask, a mixture of the aldehyde **I** (1.74 g, 5.0 mmol), 4-fluoroaniline (0.56 g,

5.0 mmol) and absolute ethanol (40 mL) was refluxed for 3 h with stirring. 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 (1.84 g, 74%).



Melting point: 95.4 °C

MS (EI): $m/z = 497$ (M^+)

IR (KBr, cm^{-1}): 3454 (O-H), 2954, 2918, 2849 (C-H aliphatic); 1758 (C=O ester); 1624 (C=N); 1609, 1510 (C=C aromatic), 1245 (C-F).

^1H NMR (400 MHz, CDCl_3): δ/ppm 0.89 (t, 3H, $J = 7.0$ Hz, CH_3), 1.28-1.45 {m, 28H, $\text{CH}_3(\text{CH}_2)_{14-}$ }, 1.74 (quint, 2H, $J = 7.3$ Hz, $-\text{CH}_2\text{CH}_2\text{COO}-$), 2.56 (t, 2H, $J = 7.5$ Hz, $-\text{CH}_2\text{COO}-$), 6.71 (dd, 1H, $J = 2.2, 8.4$ Hz, Ar-H), 6.78 (d, 1H, $J = 2.2$ Hz, Ar-H), 7.10 (m, 2H, Ar-H), 7.25 (m, 2H, Ar-H), 7.38 (d, 1H, $J = 8.4$ Hz, Ar-H), 8.58 (s, 1H, $\text{CH}=\text{N}$), 13.39 (s, 1H, OH).

^{13}C NMR (100 MHz, CDCl_3): δ/ppm 172.1 (COO), 162.8 ($\text{CH}=\text{N}$), 161.9, 160.9, 155.0, 144.8, 133.5, 123.0, 117.4, 116.7, 113.3, 110.8 (aromatic carbons), 34.8 ($-\text{CH}_2\text{COO}-$), 25.3 ($-\text{CH}_2\text{CH}_2\text{COO}-$), 32.3, 30.1, 30.0, 29.9, 29.8, 29.7, 29.6, 29.5, 23.1 ($\text{CH}_3(\text{CH}_2)_{14-}$), 14.5 (CH_3).

Elemental analysis: Calculated for $\text{C}_{31}\text{H}_{44}\text{FNO}_3$ C, 74.81%, H, 8.91%, N, 2.81%; Found: C, 74.92%, H, 8.98%, N, 2.70%.

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