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Short Note

4-{[(4-Fluorophenyl)imino]methyl}-3-hydroxyphenyl 4-(Hexadecanoyloxy)benzoate

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Abstract: A new Schiff base ester, 4-{[(4-fluorophenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate was synthesized and its IR, ^{1}H NMR, ^{13}C NMR and EI-MS spectroscopic data are presented.

Keywords: Schiff base; liquid crystal; 4-{[(4-fluorophenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate

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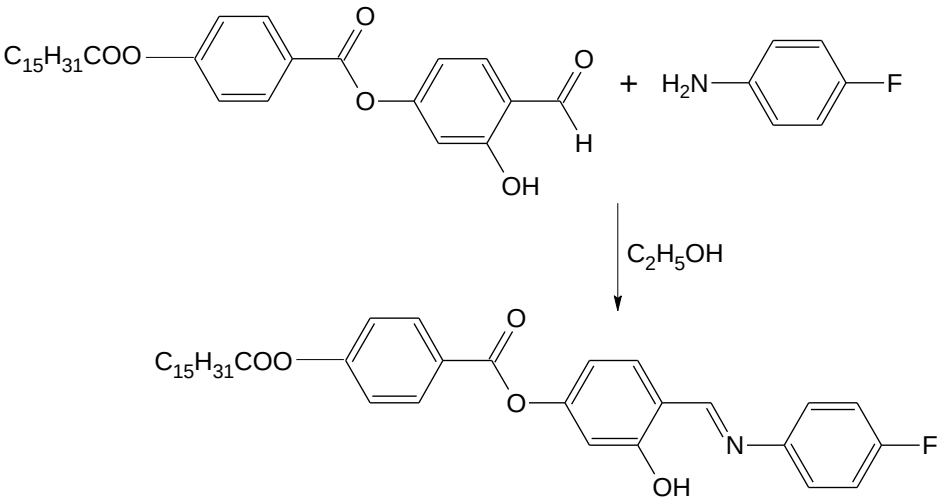
Schiff bases have attracted much attention from many researchers owing to their thermochromic and photochromic properties [1–5]. The presence of a long alkyl chain at the *para* position of the aldehyde or aniline fragment of *N*-benzylideneanilines has also been identified as one of the important requirements which favours the existence of liquid crystal phases [6–8]. Different alkyl chain length and terminal substituent can significantly influence the anisotropic properties of liquid crystals [6]. Thus, we report here another new derivative containing an hexadecanoyloxy chain, 4-{[(4-fluorophenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.

Scheme 1. Synthesis of 4-{[(4-Fluorophenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.



Experimental

Analytical data were obtained on Perkin Elmer 2400 LS series CHNS/O analyzers. Electron impact mass spectra (EI-MS) were recorded by Hewlett Packard 5989A Mass Spectrometer operating at 70 eV ionizing energy. FT-IR data were recorded on a Perkin Elmer 2000-FTIR spectrophotometer. NMR spectra were recorded in $CDCl_3$ on a Bruker 400 MHz Ultrashield Spectrometer.

4-(4-*n*-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehye was prepared according to method described in our previous work [9]. In a round-bottom flask, a mixture of the aldehyde (2.48 g, 5.0 mmol), 4-fluoroaniline (0.56 g, 5.0 mmol) and absolute ethanol (40 mL) was refluxed with stirring for 3 h. 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 (1.56 g, 53%).

Melting point: 189–191 ℃

MS (EI): *m/z* (rel. int. %) = 590 (1) (M^+).

IR (KBr): ν_{max} (cm^{-1}), 2953, 2916, 2848 (C-H aliphatic), 1755 (C=O of $C_{15}H_{31}COO$- fragment), 1743 (C=O of benzoate), 1625 (C=N), 1605 (C=C aromatic), 1282 (C-O).

^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm, 0.91 (t, 3H, *J* = 6.8 Hz, C<u>H</u>$_3$-), 1.24–1.47 (m, 24H, CH_3-(C<u>H</u>$_2$)$_{12}$-), 1.79 (quint, 2H, *J* = 7.5 Hz, -C<u>H</u>$_2$-CH_2COO-), 2.62 (t, 2H, *J* = 7.5 Hz, -C<u>H</u>$_2$-COO-), 6.86 (dd, 1H, *J* = 2.2, 8.4 Hz, Ar-<u>H</u>), 6.93 (d, 1H, *J* = 2.2 Hz, Ar-H), 7.12–7.17 (m, 2H, Ar-H), 7.26–7.31 (m, 4H, Ar-H), 7.46 (d, 1H, *J* = 8.5 Hz, Ar-H), 8.25 (d, 2H, *J* = 8.8 Hz, Ar-H), 8.62 (s, 1H, CH=N), 13.45 (s, 1H, OH).

^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm, 171.86 (C=O of $C_{15}H_{31}$<u>C</u>OO-), 164.11 (C=O of benzoate), 163.27 (C=N), 162.94, 161.94, 155.64, 155.14, 144.93, 133.54, 132.17, 127.08, 122.92, 122.25, 117.62, 116.49, 113.33 and 110.95 for aromatic carbons, 34.81 (-<u>C</u>H_2COO-), 25.28 (-<u>C</u>H_2CH_2COO-),

32.27, 30.03, 30.02, 30.00, 29.98, 29.94, 29.79, 29.68, 29.58, 29.46, 23.01 ($CH_3(\underline{C}H_2)_{12}$), 14.37 ($\underline{C}H_3(CH_2)_{12}$).

Elemental analysis: Calculated for $C_{36}H_{44}NO_5F$, 73.32%, H, 7.52%, N, 2.38%; Found: C, 73.37%, H, 7.50%, N, 2.40%.

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