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Short Note

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

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

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

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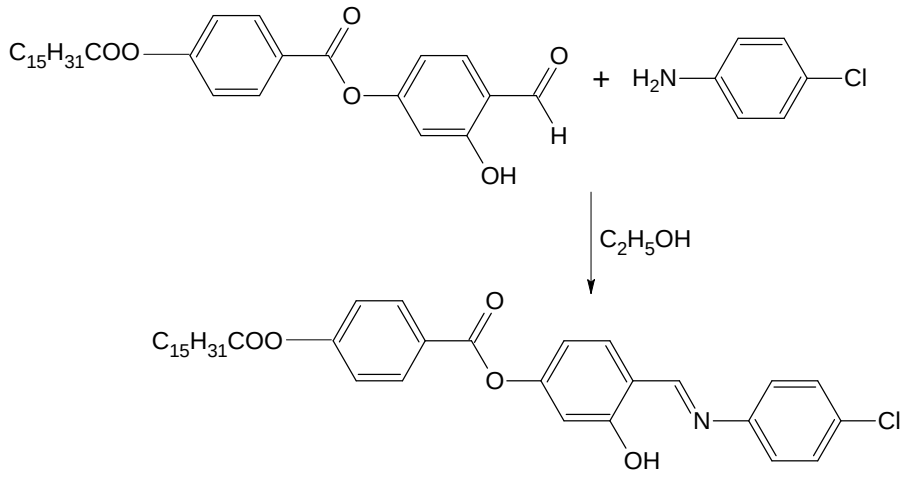
Benzylideneanilines (Schiff bases) exhibit very interesting thermochromic and photochromic properties. Therefore, they became a topic of numerous recent publications [1–6]. Flexible long alkyl chain at the *para* position of *N*-benzylideneanilines has also been viewed as one of the important criteria for exhibition of liquid crystal phases [7–10]. Different alkyl chain length and terminal substituent can significantly influence the anisotropic properties of liquid crystals [7,8]. Thus, we report here another new derivative containing an hexadecanoyloxy chain, 4-{[(4-chlorophenyl)imino] methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.

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



Experimental

4-(4-*n*-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehye was prepared according to method that described in our previous work [11]. In a round-bottom flask, a mixture of the aldehyde (2.48 g, 5.0 mmol), 4-chloroaniline (0.64 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 (1.88 g, 62%).

Melting point: 214–215 °C.

MS (EI): *m/z* (rel. int. %) = 606 (1) (M^+).

IR (KBr): ν_{max}/ cm^{-1} 3400 (broad, O-H), 2951, 2916, 2848 (C-H aliphatic), 1755 (C=O of $C_{15}H_{31}COO$-fragment), 1743 (C=O of benzoate), 1625 (C=N), 1604 (C=C aromatic), 1282 (C-O).

^{1}H-NMR (400 MHz, $CDCl_3$): δ/ppm 0.92 (t, 3H, *J* = 6.7 Hz, C$\underline{H}_3$-), 1.25–1.53 (m, 24H, CH_3-(C$\underline{H}_2$)$_{12}$-), 1.80 (quint, 2H, *J* = 7.4 Hz, -C$\underline{H}_2$-CH_2COO-), 2.62 (t, 2H, *J* = 7.5 Hz, -C$\underline{H}_2$-COO-), 6.87 (dd, 1H, *J* = 2.2, 8.4 Hz, Ar-$\underline{H}$), 6.94 (d, 1H, *J* = 2.1 Hz, Ar-H), 7.23–7.29 (m, 4H, Ar-H), 7.40–7.43 (m, 2H, Ar-H), 7.45 (d, 1H, *J* = 8.4 Hz, Ar-H), 8.25 (d, 2H, *J* = 8.6 Hz, Ar-H), 8.63 (s, 1H, CH=N), 13.26 (s, 1H, OH).

^{13}C-NMR (100 MHz, $CDCl_3$): δ/ppm 171.9 (C=O of $C_{15}H_{31}\underline{C}$OO-), 164.3 (C=O of benzoate), 162.5 (C=N), 163.0, 155.7, 155.3, 147.3, 133.7, 133.1, 132.2, 130.0, 127.1, 122.8, 122.3, 117.6, 113.4 and 111.0 for aromatic carbons, 34.8 (-$\underline{C}H_2$COO-), 25.2 (-$\underline{C}H_2CH_2$COO-), 32.3, 30.1, 30.0, 29.9, 29.8, 29.7, 29.6, 29.5, 23.0 (CH_3($\underline{C}H_2$)$_{12}$), 14.4 ($\underline{C}H_3$(CH_2)$_{12}$).

Elemental analysis: Calculated for $C_{36}H_{44}NO_5Cl$, 71.33%, H, 7.32%, N, 2.31%; Found: C, 71.36%, H, 7.30%, N, 2.32%.

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