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Short Note

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

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Abstract: A new Schiff base, 4-{[(4-methylphenyl)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-methylphenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate

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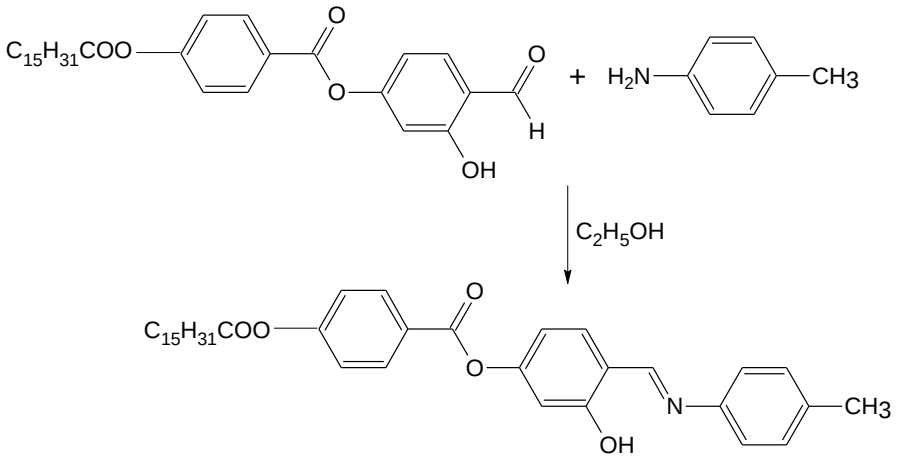
N-Benzylideneaniline Schiff bases have received a considerable amount of attention from many researchers owing to their importance in exhibiting thermochromism and photochromism [1]. A lot of efforts have been made in order to generate their derivatives by introducing different substituents into the existing skeleton of the molecule The presence of alkyl chain at the *para* position of *N*-benzylideneanilines has also been identified as one of the important requirements which favours the existence of liquid crystal phases [2-4]. Different alkyl chain length and terminal substituent can significantly influence the anisotropic properties of liquid crystals [2]. Thus, we report here another new derivative containing an hexadecanoyloxy chain, 4-{[(4-methylphenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.

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



Experimental

4-(4-*n*-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehye was prepared according to the method described in our previous work [5]. In a round-bottom flask, a mixture of the aldehyde (2.48 g, 5.0 mmol), 4-methylaniline (0.54 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 (2.20 g, 75%).

Melting point: 204–206 ℃.

MS (EI): *m/z* (rel. int. %) = 586 (1) (M^+).

IR (KBr): ν_{max}/ cm^{-1} 2952, 2916, 2848 (C-H aliphatic), 1752 (C=O of $C_{15}H_{31}COO$- fragment), 1743 (C=O of benzoate), 1624 (C=N), 1605 (C=C aromatic), 1284 (C-O).

^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 0.88 (t, 3H, *J* = 6.4 Hz, C$\underline{H}_3$-), 1.24–1.47 (m, 24H, CH_3-(C$\underline{H}_2$)$_{12}$-), 1.77 (quint, 2H, *J* = 7.3 Hz, -C$\underline{H}_2$-CH_2COO-), 2.38 (s, 1H, Ar-CH_3), 2.60 (t, 2H, *J* = 7.5 Hz, -C$\underline{H}_2$-COO-), 6.81 (dd, 1H, *J* = 2.2, 8.4 Hz, Ar-H), 6.89 (d, 1H, *J* = 2.1 Hz, Ar-H), 7.21–7.26 (m, 6H, Ar-H), 7.42 (d, 1H, *J* = 8.5 Hz, Ar-H), 8.23 (d, 2H, *J* = 8.8 Hz, Ar-H), 8.63 (s, 1H, CH=N), 13.77 (s, 1H, OH).

^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 172.06 (C=O of $C_{15}H_{31}\underline{C}$OO-), 164.26 (C=O of benzoate), 161.17 (C=N), 163.03, 155.52, 154.77, 145.95, 137.45, 133.44, 132.26, 130.45, 127.07, 122.33, 121.40, 117.81, 113.22 and 110.94 for aromatic carbons, 34.83 (-$\underline{C}H_2$COO-), 25.25 (-$\underline{C}H_2CH_2$COO-), 21.47 (Ar-$\underline{C}H_3$), 32.34, 30.11, 30.09, 30.06, 30.01, 29.86, 29.77, 29.66, 29.50, 23.11 (CH_3($\underline{C}H_2$)$_{12}$), 14.53 ($\underline{C}H_3$(CH_2)$_{12}$).

Elemental analysis: Calculated for $C_{37}H_{47}NO_5$, C 75.86%, H, 8.09%, N, 2.39%; Found: C, 75.88%, H, 8.08%, N, 2.45%.

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