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Short Note

3-Hydroxy-4-[(phenylimino)methyl]phenyl 4-(Hexadecanoyloxy) benzoate

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

Keywords: Schiff base; mesomorphic; 3-hydroxy-4-[(phenylimino)methyl]phenyl 4-(hexadecanoyloxy)benzoate

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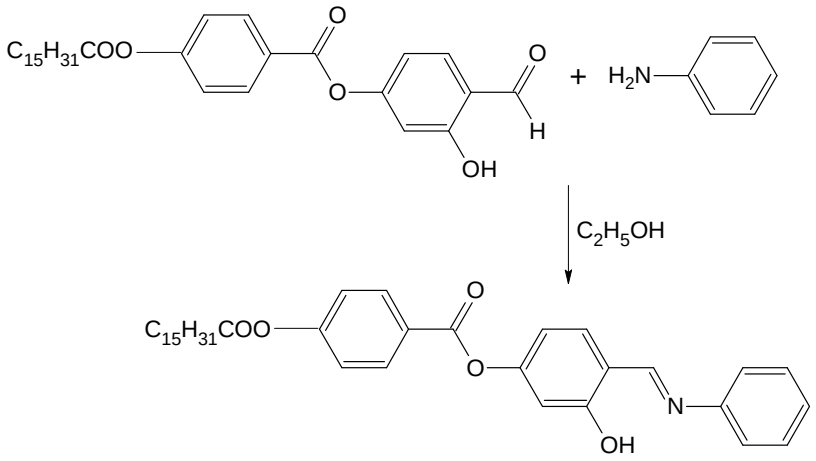
Mesomorphic materials have many practical applications, in particular as display devices, organic light emitting diodes, anisotropic networks, photoconductors and semiconductor materials [1–3]. Strong demand of new mesomorphic compounds for applications has encouraged the synthesis and study of numerous mesogens in particular, thermotropic liquid crystals [4,5]. Wide-ranging research on Schiff base core systems has been carried out since the discovery of MBBA, which exhibited room temperature nematic phase [6]. Several studies have been conducted on ester type of Schiff bases due to their interesting properties and substantial temperature range [7–13]. Thus, we report here another new derivative containing an hexadecanoyloxy chain, 3-hydroxy-4-[(phenylimino)methyl]phenyl 4-(hexadecanoyloxy)benzoate.

Scheme 1. Synthesis of 3-hydroxy-4-[(phenylimino)methyl]phenyl 4-(hexadecanoyloxy)benzoate.



Experimental

4-(4-*n*-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehye was prepared according to a method that was described in our previous work [13]. In a round-bottom flask, a mixture of the aldehyde (2.48 g, 5.0 mmol), aniline (0.47 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 (1.14 g, 40%).

Melting point: 153–154 °C

MS (EI): *m/z* (rel. int. %) = 572 (1) (M^+).

IR (KBr): ν_{max}/ cm^{-1} 2953, 2916, 2848 (C-H aliphatic), 1752 (C=O of $C_{15}H_{31}COO$- fragment), 1743 (C=O of benzoate), 1628 (C=N), 1605 (C=C aromatic), 1283 (C-O).

^{1}H-NMR (400 MHz, $CDCl_3$): δ/ppm 0.90 (t, 3H, *J* = 6.5 Hz, C<u>H</u>$_3$-), 1.22–1.42 (m, 24H, CH_3-(C<u>H</u>$_2$)$_{12}$-), 1.80 (quint, 2H, *J* = 7.2 Hz, -C<u>H</u>$_2$-CH_2COO-), 2.63 (t, 2H, *J* = 7.4 Hz, -C<u>H</u>$_2$-COO-), 6.86 (dd, 1H, *J* = 2.2, 8.4 Hz, Ar-<u>H</u>), 6.92 (d, 1H, *J* = 2.2 Hz, Ar-<u>H</u>), 7.26–7.34 (m, 5H, Ar-<u>H</u>), 7.40–7.48 (m, 3H, Ar-<u>H</u>), 8.26 (dd, 2H, *J* = 2.3, 8.7 Hz, Ar-<u>H</u>), 8.66 (s, 1H, C<u>H</u>=N), 13.67 (s, 1H, O-<u>H</u>).

^{13}C-NMR (100 MHz, $CDCl_3$): δ/ppm 172.09 (C=O of $C_{15}H_{31}$<u>C</u>OO-), 164.25 (C=O of benzoate), 162.17 (C=N), 163.0, 155.5, 155.0, 148.6, 133.6, 132.3, 129.9, 127.0, 126.8, 122.3, 121.6, 117.7, 113.3 and 111.0 for aromatic carbons, 34.8 (-<u>C</u>H_2COO-), 25.3 (-<u>C</u>H_2CH_2COO-), 32.3, 30.1, 30.0, 29.9, 29.8, 29.7, 29.5, 23.1 (CH_3(<u>C</u>H_2)$_{12}$), 14.5 (<u>C</u>H_3(CH_2)$_{12}$).

Elemental analysis: Calculated for $C_{36}H_{45}NO_5$, 75.63%, H, 7.93%, N, 2.45%; Found: C, 75.66%, H, 7.91%, N, 2.44%.

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