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Short Note

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

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

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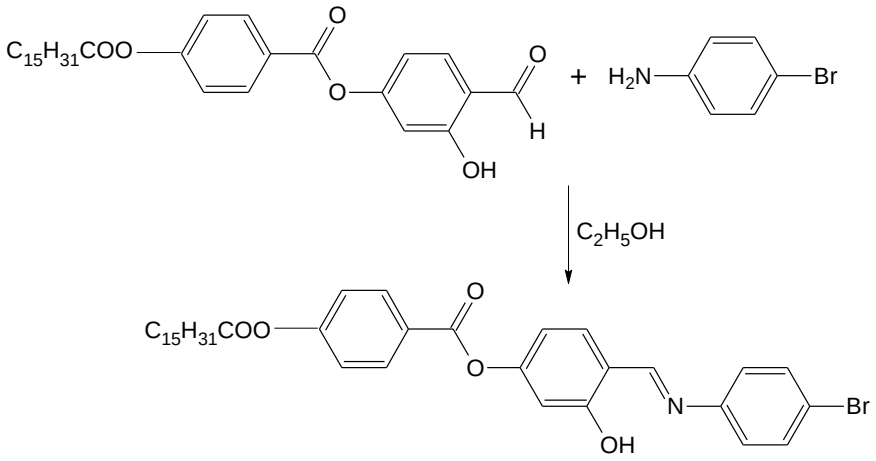
High demand for new liquid crystals (LCs) for applications has led to the preparation and study of numerous mesogens in particular, thermotropic liquid crystals [1,2]. Most thermotropic liquid crystals are calamitic molecules having a rigid core composed of two or more phenyl rings and one or more flexible terminal alkyl chains. Schiff base, also known as imine (CH=N), is one of the most well-known linking groups used in connecting the rigid core groups. Wide-ranging research on Schiff base core systems has been conducted since the discovery of MBBA which exhibited room temperature nematic phase [3]. Several studies have been conducted on ester-type Schiff bases owing to their interesting properties and substantial temperature range [4–9]. As a continuation of our previous work, we report here a new liquid crystal, 4-{[(4-bromophenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.

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



Experimental

4-(4-*n*-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehye was prepared according to a method that we described in our previous work [10]. In a round-bottom flask, a mixture of the aldehyde (2.48 g, 5.0 mmol), 4-bromoaniline (0.86 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 (1.50 g, 46%).

Melting point: 222–224 ℃

MS (EI): *m/z* (rel. int. %): 651 (M^+, 1).

IR (KBr): ν_{max}/ cm^{-1} 2950, 2916, 2848 (C-H aliphatic), 1754 (C=O of $C_{15}H_{31}COO$- fragment), 1743 (C=O of benzoate), 1623 (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$\underline{H}_3$-), 1.24–1.45 (m, 24H, CH_3-(C$\underline{H}_2$)$_{12}$-), 1.80 (quint, 2H, *J* = 7.4 Hz, -C$\underline{H}_2$-CH_2COO-), 2.63 (t, 2H, *J* = 7.5 Hz, -C$\underline{H}_2$-COO-), 6.87 (dd, 1H, *J* = 2.1, 8.4 Hz, Ar-$\underline{H}$), 6.93 (d, 1H, *J* = 2.0 Hz, Ar-H), 7.20 (d, 2H, *J* = 8.6 Hz, Ar-H), 7.28 (d, 2H, *J* = 8.7 Hz, Ar-H), 7.47 (d, 1H, *J* = 8.5 Hz, Ar-H), 7.58 (d, 2H, *J* = 8.6 Hz, Ar-H), 8.26 (d, 2H, *J* = 8.7 Hz, Ar-H), 8.64 (s, 1H, CH=N), 13.20 (s, 1H, OH).

^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 172.18 (C=O of $C_{15}H_{31}\underline{C}OO$-), 164.26 (C=O of benzoate), 162.56 (C=N), 162.96, 155.55, 155.17, 147.64, 133.83, 132.97, 132.31, 126.94, 123.26, 122.40, 120.94, 117.56, 113.58 and 111.08 for aromatic carbons, 34.83 (-$\underline{C}H_2$COO-), 25.25 (-$\underline{C}H_2CH_2$COO-), 32.36, 30.13, 30.11, 30.09, 30.08, 30.03, 29.88, 29.80, 29.68, 29.52, 29.43, 23.13 (CH_3($\underline{C}H_2$)$_{12}$), 14.58 ($\underline{C}H_3$(CH_2)$_{12}$).

Elemental analysis: Calculated for $C_{36}H_{44}NO_5Br$, 66.46%, H, 6.82%, N, 2.15%; Found: C, 66.44%, H, 6.87%, N, 2.17%.

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