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, 1H NMR, 13C NMR and MS spectroscopic data are presented.

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

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.

Experimental

4-(4-n-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehyde 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 °C.

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, CH_{3}-), 1.24–1.47 (m, 24H, CH_{3}(CH_{2})_{12}-), 1.77 (quint, 2H, J = 7.3 Hz, -CH_{2}-CH_{2}COO-), 2.38 (s, 1H, Ar-CH_{3}), 2.60 (t, 2H, J = 7.5 Hz, -CH_{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}COO-), 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 (-CH_{2}COO-), 25.25 (-CH_{2}CH_{2}COO-), 21.47 (Ar-CH_{3}), 32.34, 30.11, 30.09, 30.06, 30.01, 29.86, 29.77, 29.66, 29.50, 23.11 (CH_{3}(CH_{2})_{12}), 14.53 (CH_{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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References


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