Molbank **2012**, M753; doi:10.3390/M753

OPEN ACCESS

molbank

ISSN 1422-8599

www.mdpi.com/journal/molbank

Short Note

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

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Received: 27 February 2012 / Accepted: 9 April 2012 / Published: 17 April 2012

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

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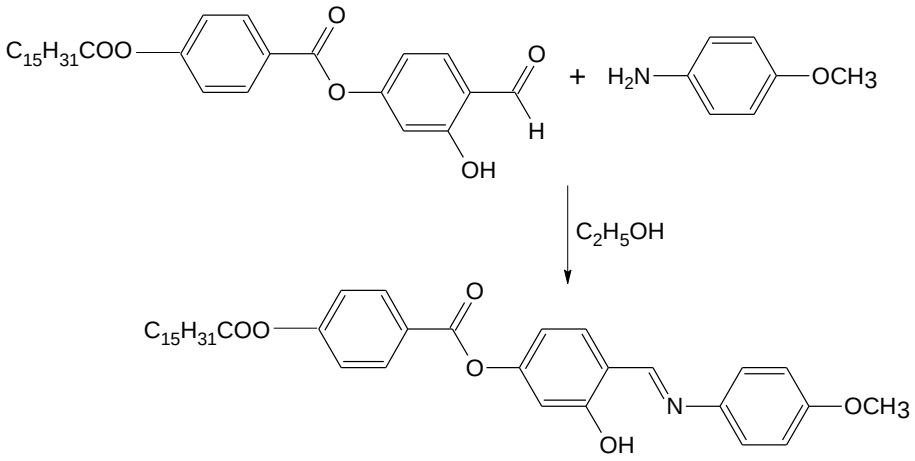
Much attention has been focused on Schiff base derivatives owing to their thermochromic and photochromic properties [1–5]. Schiff bases are also well recognized for their liquid crystal properties since the discovery of MBBA which exhibited room temperature nematic phase [6]. An appropriate length of the alkyl chain at the *para* position of the aldehyde or aniline fragment of *N*-benzylidene-anilines has also been identified as one of the main requirements which favours the existence of liquid crystal phase (or mesophase) [7–9]. Different terminal substituents can also significantly influence the anisotropic properties of liquid crystals [7]. In this continuation work, we report here a new liquid crystal, 4-{[(4-methoxyphenyl)imino]methyl}-3-hydroxyphenyl 4-(hexadecanoyloxy)benzoate.

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



Experimental

4-(4-*n*-Hexadecanoyloxybenzoyloxy)-2-hydroxybenzaldehye was prepared according to a method that was described in our previous work [10]. In a round-bottom flask, a mixture of the aldehyde (2.48 g, 5.0 mmol), 4-methoxyaniline (0.62 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 (2.08 g, 69%).

Melting point: 221–222 ℃.

MS (EI): *m/z* (rel. int. %) = 602 (1) (M^+).

IR (KBr): ν_{max}/ cm^{-1} 2953, 2916, 2848 (C-H, aliphatic), 1753 (C=O of $C_{15}H_{31}COO$- fragment), 1742 (C=O of phenyl benzoate), 1624 (C=N), 1605 (C=C, aromatic), 1284 (C-O).

^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 0.90 (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* = 7.6 Hz, -C$\underline{H}_2$-CH_2COO-), 2.63 (t, 2H, *J* = 7.4 Hz, -C$\underline{H}_2$-COO-), 3.88 (s, 3H, Ar-OCH_3), 6.84 (dd, 1H, *J* = 2.1, 8.3 Hz, Ar-H), 6.91 (d, 1H, *J* = 2.1 Hz, Ar-H), 6.99 (d, 2H, *J* = 8.8 Hz, Ar-H), 7.26–7.31 (m, 4H, Ar-H), 7.45 (d, 1H, *J* = 8.5 Hz, Ar-H), 8.26 (d, 2H, *J* = 8.7 Hz, Ar-H), 8.65 (s, 1H, CH=N), 13.83 (s, 1H, OH).

^{13}C NMR (100 MHz, $CDCl_3$): 172.09 (C=O of $C_{15}H_{31}\underline{C}OO$-), 164.31 (C=O of phenyl benzoate), 159.94 (C=N), 162.87, 159.33, 155.51, 154.48, 144.90, 133.25, 132.26, 127.05, 122.70, 122.32, 117.60, 115.06, 113.19 and 110.90 for aromatic carbons, 55.96 (Ar-O$\underline{C}H_3$), 34.83 (-$\underline{C}H_2$COO-), 25.25 (-$\underline{C}H_2CH_2$COO-), 32.33, 30.10, 30.06, 30.00, 29.85, 29.76, 29.65, 29.50, 23.10 (CH_3(C$\underline{H}_2$)$_{12}$), 14.52 ($\underline{C}H_3$(CH_2)$_{12}$).

Elemental analysis: Calcd. for $C_{37}H_{47}NO_6$, 73.85%, H, 7.87%, N, 2.33%; Found: C, 73.90%, H, 7.86%, N, 2.30%.

Acknowledgements

Authors would like to thank Universiti Tunku Abdul Rahman and Universitit Sains Malaysia for the financial supports and research facilities.

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