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Short Note

3-Hydroxy-4-{[(4-ethylphenyl)imino]methyl}phenyl Octadecanoate

Sie-Tiong Ha [1,*], Jun-Kit Beh [2], Yip-Foo Win [1] and Siew-Teng Ong [1]

[1] Department of Chemical Science, Faculty of Science, Universiti Tunku Abdul Rahman, Jln Universiti, Bandar Barat, 31900 Kampar, Perak, Malaysia

[2] Department of Science, Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, Jln Genting Jelang, Setapak, 53300 Kuala Lumpur, Malaysia

* Author to whom correspondence should be addressed; E-Mail: hast@utar.edu.my or hast_utar@yahoo.com.

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

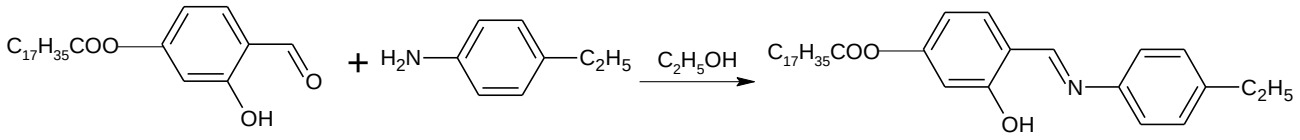
Keywords: 3-hydroxy-4-{[(4-ethylphenyl)imino]methyl}phenyl octadecanoate; Schiff base; alkyl chain

The mesomorphic behavior of an organic compound is basically dependent on its molecular architecture in which a slight change in the molecular geometry brings about considerable change in its mesomorphic properties. Many mesogenic homologous series contain two central linkages, both of which may either be ester [1] or Schiff base (CH=N) linking groups [2] or one of which may be an ester and the other one a Schiff base [3]. Schiff base esters possessing a long alkyl chain have received overwhelming attention due to their possibility to show liquid crystallinity properties such as smectic and nematic phases [4–7].

Synthesis

4-Formyl-3-hydroxyphenyl octadecanoate was previously prepared *via* Steglich esterification [8]. In a round-bottom flask, a mixture of the aldehyde (1.74 g, 5.0 mmol), 4-ethylaniline (0.61 g,

5.0 mmol) and absolute ethanol (40 mL) was refluxed for 3h with stirring. 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 (0.96 g, 39%).



Melting point: 86.2 ^{o}C

MS (EI): *m/z* = 507 (M^{+})

IR (KBr, cm^{-1}): 3448 (O-H), 2955, 2917, 2848 (C-H aliphatic); 1758 (C=O ester); 1628 (C=N); 1607, 1472 (C=C aromatic).

^{1}H NMR (400 MHz, $CDCl_3$): δ/ppm 0.91 (t, 3H, *J* = 7.1 Hz, CH_3), 1.27 (t, 3H, *J* = 7.3 Hz, Ar-CH_2-$C\underline{H}_3$), 1.28-1.46 {m, 28H, $CH_3(C\underline{H}_2)_{14}$-}, 1.78 (quint, 2H, *J* = 7.5 Hz, -$C\underline{H}_2CH_2COO$-), 2.58 (t, 2H, *J* = 7.4 Hz, -$C\underline{H}_2COO$-), 2.70 (q, 2H, *J* = 7.6 Hz, Ar-$C\underline{H}_2CH_3$), 6.70 (dd, 1H, *J* = 2.2, 8.4 Hz, Ar-H), 6.77 (d, 1H, *J* = 2.2 Hz, Ar-H), 7.22-7.28 (m, 4H, Ar-H), 7.38 (d, 1H, *J* = 8.4 Hz, Ar-H), 8.63 (s, 1H, CH=N), 13.71 (s, 1H, OH).

^{13}C NMR (100 MHz, $CDCl_3$): δ/ppm 172.1 (COO), 161.2 (CH=N), 163.0, 154.8, 146.2, 143.8, 133.3, 129.2, 121.4, 117.6, 113.1, 110.8 (aromatic carbons), 34.9 (-$\underline{C}H_2COO$-), 25.3 (-$\underline{C}H_2CH_2COO$-), 28.9 (Ar-$\underline{C}H_2CH_3$), 32.3, 30.1, 30.0, 29.9, 29.8, 29.7, 29.6, 29.5, 23.1 ($CH_3(\underline{C}H_2)_{14}$-), 16.0 (Ar-$CH_2C\underline{H}_3$), 14.5 ($C\underline{H}_3(CH_2)_{14}$).

Elemental analysis: Calculated for $C_{33}H_{49}NO_3$ C, 78.06%, H, 9.73%, N, 2.76%; Found: C, 78.18%, H, 9.65%, N, 2.71%.

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