

Short Note

4-{[(4-Iodophenyl)imino]methyl}phenyl Octadecanoate

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

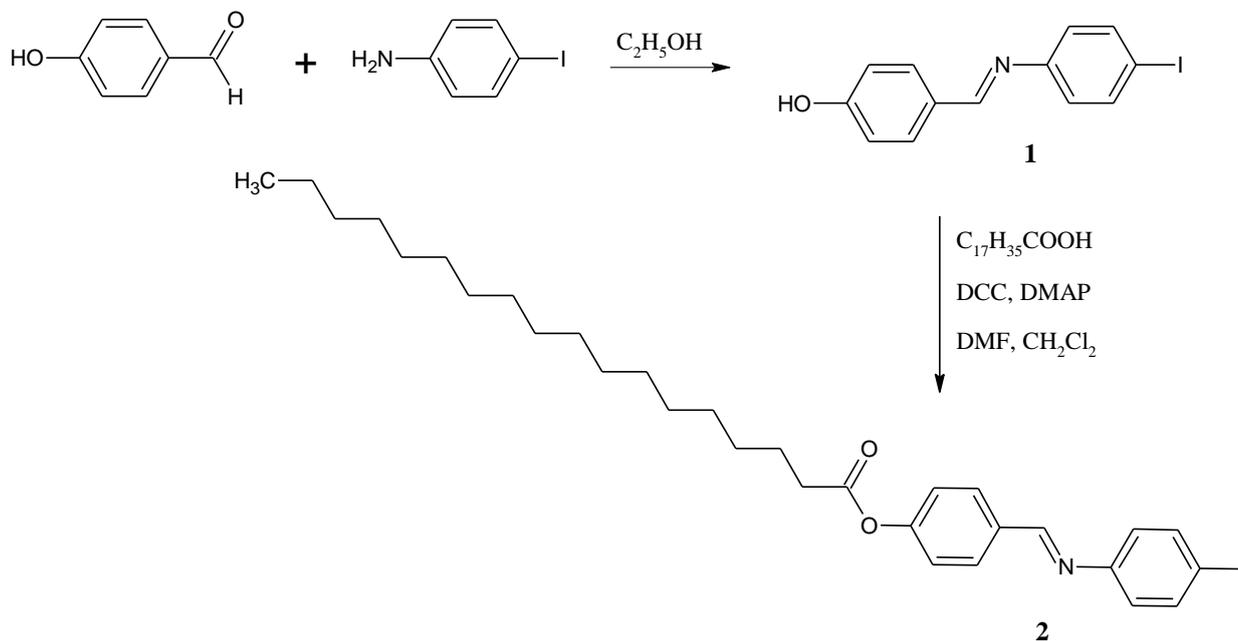
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Liquid crystalline materials have many practical applications in scientific and technological areas, in particular as display devices, organic light emitting diodes, anisotropic networks, photoconductors and semiconductor materials [1-3]. High demand of new liquid crystals for applications has led to the preparation and study of numerous mesogens in particular, thermotropic liquid crystals [4,5]. In our previous studies, the results revealed that azomethine and ester groups are useful connecting units for generating mesomorphism in thermotropic liquid crystals with two and three aromatic rings. Aromatic azomethine ester comprising of different polarity of substituents has been known to either promote or suppress the mesomorphic properties [6-8]. As a continuation of our previous work, Schiff base esters and iodo terminal moieties are incorporated to form a new compound, 4-{[(4-iodophenyl)imino]methyl}phenyl octadecanoate.

Experimental

Analytical data were obtained on Perkin Elmer 2400 LS series CHNS/O analyzers. Electron impact mass spectra (EI-MS) were recorded by Hewlett Packard 5989A Mass Spectrometer operating at 70 eV ionizing energy. FT-IR data were recorded on a Perkin Elmer 2000-FTIR spectrophotometer. NMR spectra were recorded in CDCl_3 on a Bruker 400 MHz Ultrashield Spectrometer.

Scheme 1. Synthesis of 4-[[[4-iodophenyl]imino]methyl]phenyl octadecanoate.



In analogy to a recently published procedure [9-12], a solution of 4-hydroxybenzaldehyde (1.22 g, 10 mmol) and 4-iodoaniline (2.19 g, 10 mmol) in absolute ethanol (70 mL) was heated under reflux for 3 h. Schiff base **1** thus obtained was recrystallized from absolute ethanol. Then, Schiff base **1** (0.66 g, 2 mmol) in dimethylformamide (DMF) (2 mL), was added into a solution of octadecanoic acid (0.57 g, 2 mmol) and 4-dimethylaminopyridine (DMAP) (0.12 g, 1 mmol) in dichloromethane (20 mL). The resulting mixture was stirred in an ice bath. To this solution, N,N' -dicyclohexylcarbodiimide (DCC) (0.41 g, 2 mmol) dissolved in dichloromethane (5 mL) was added dropwise while stirring in the ice bath for 1 h. The resulting mixture was subsequently stirred at room temperature for another 3 h. Then, the reaction mixture was filtered and the excess solvent was removed from the filtrate by evaporation. Recrystallization from absolute ethanol gave the Schiff base **2** as pale yellow solid (0.814 g, 69%).

Melting point: 109–110 °C.

MS (EI): m/z (rel. int. %) = 589 (8) (M^+), 323 (100).

IR (KBr): ν_{max} (cm^{-1}), 2954, 2915, 2849 (C-H aliphatic), 1753 (C=O), 1617 (C=N), 1215, 1101 (C-O).

^1H NMR (400 MHz, CDCl_3): δ /ppm 0.90 (t, 3H, $J = 6.6\text{ Hz}$, CH_3 -), 1.28 (m, 16H, CH_3 - $(\text{CH}_2)_{14}$ -), 1.78 (qt, 2H, $J = 7.4\text{ Hz}$, $-\text{CH}_2\text{-CH}_2\text{-COO-}$), 2.60 (t, 2H, $J = 7.5\text{ Hz}$, $-\text{CH}_2\text{-COO-}$), 6.98 (d, 2H, $J = 8.7\text{ Hz}$,

Ar-H), 7.22 (d, $J = 8.4$ Hz, 2H, Ar-H), 7.72 (d, $J = 8.7$ Hz, 2H, Ar-H), 7.93 (d, $J = 8.4$ Hz, 2H, Ar-H), 8.67 (s, 1H, -CH=N-).

^{13}C NMR (100 MHz, CDCl_3): δ/ppm 14.10 ($\underline{\text{C}}\text{H}_3$ -), 22.68 ($\text{CH}_3\underline{\text{C}}\text{H}_2$ -), 24.88 ($\text{CH}_3\text{CH}_2\underline{\text{C}}\text{H}_2$ -), 29.10, 29.24, 29.35, 29.45, 29.59, 29.65, 29.69 for methylene carbons ($\text{CH}_3\text{CH}_2\text{CH}_2$ -($\underline{\text{C}}\text{H}_2$) $_{12}$ -), 31.92 ($\underline{\text{C}}\text{H}_2\text{CH}_2\text{COO}$ -), 34.43 ($\underline{\text{C}}\text{H}_2\text{COO}$ -), 90.32, 122.10, 122.93, 130.07, 133.51, 138.19, 151.57, 153.37 for aromatic carbons, 159.50 ($\underline{\text{C}}\text{H}=\text{N}$ -), 171.87 ($\underline{\text{C}}\text{OO}$ -).

Elemental analysis: Calculated for $\text{C}_{31}\text{H}_{44}\text{INO}_2$, 63.15%, H, 7.52%, N, 2.38%; Found: C, 63.21%, H, 7.42%, N, 2.31%.

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