

Short Note

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

Sie-Tiong Ha <sup>1,\*</sup>, Mei-Yoke Ng <sup>2</sup>, Teck-Ming Koh <sup>2,†</sup> and Teck-Leong Lee <sup>1,2</sup>

<sup>1</sup> Department of Chemical Science, Faculty of Science, Universiti Tunku Abdul Rahman, Jln Universiti, Bandar Barat, 31900 Kampar, Perak, Malaysia

<sup>2</sup> Department of Science, Faculty of Engineering and Science, Universiti Tunku Abdul Rahman, Jln Genting Jelang, Setapak, 53300 Kuala Lumpur, Malaysia

† Present address: Department of Chemistry, National University of Singapore, 3 Science Drive 3, Singapore 117543.

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

Received: 25 March 2010 / Accepted: 8 April 2010 / Published: 9 April 2010

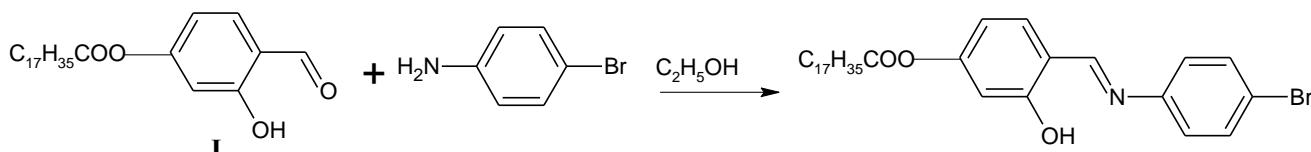
**Abstract:** A new Schiff base ester, 3-hydroxy-4-{[(4-bromophenyl)imino]methyl}phenyl octadecanoate, was synthesized and its IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR and MS spectroscopic data are presented.

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

Schiff bases have attracted overwhelming attentions from many researchers owing to their importance in exhibiting thermochromism and photochromism [1–4]. The presence of a long alkyl chain at the *para* position of the aldehyde or aniline fragment of *N*-benzylideneanilines has been regarded as one of the important elements which favours the existence of liquid crystal phases [5–7]. Different terminal chain length can significantly influence the anisotropic properties of liquid crystals [5]. Thus, we report here another new derivative containing an octadecanoyloxy chain, 3-hydroxy-4-{[(4-bromophenyl)imino]methyl}phenyl octadecanoate.

## Synthesis

4-Formyl-3-hydroxyphenyl octadecanoate was previously prepared *via* Steglich esterification [8]. In a round-bottom flask, a mixture of the aldehyde **I** (1.74 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 (1.06 g, 38%).



Melting point: 110.1 °C

MS (EI):  $m/z = 558 (M^+)$

IR (KBr,  $\text{cm}^{-1}$ ): 3447 (O-H), 2950, 2917, 2848 (C-H aliphatic); 1758 (C=O ester); 1629 (C=N); 1607, 1471 (C=C aromatic), 1075 (C-Br).

$^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ ):  $\delta/\text{ppm}$  0.92 (t, 3H,  $J = 7.2$  Hz,  $\text{CH}_3$ ), 1.29-1.49 {m, 28H,  $\text{CH}_3(\text{CH}_2)_{14}-$ }, 1.79 (quint, 2H,  $J = 7.3$  Hz,  $-\text{CH}_2\text{CH}_2\text{COO}-$ ), 2.57 (t, 2H,  $J = 7.4$  Hz,  $-\text{CH}_2\text{COO}-$ ), 6.72 (dd, 1H,  $J = 2.2, 8.4$  Hz, Ar-H), 6.79 (d, 1H,  $J = 2.1$  Hz, Ar-H), 7.16 (dd, 2H,  $J = 2.7, 8.6$  Hz, Ar-H), 7.36 (d, 1H,  $J = 8.5$  Hz, Ar-H), 7.54 (dd, 2H,  $J = 2.7, 8.6$  Hz, Ar-H), 8.58 (s, 1H,  $\text{CH}=\text{N}$ ), 13.13 (s, 1H, OH).

$^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ ):  $\delta/\text{ppm}$  171.7 (COO), 163.0 (CH=N), 162.5, 155.4, 147.9, 133.5, 132.9, 123.1, 117.3, 113.3, 110.8, 110.0 (aromatic carbons), 34.83 ( $-\text{CH}_2\text{COO}-$ ), 25.25 ( $-\text{CH}_2\text{CH}_2\text{COO}-$ ), 32.24, 29.98, 29.95, 29.90, 29.75, 29.63, 29.54, 29.43, 22.95 ( $\text{CH}_3(\text{CH}_2)_{14}-$ ), 14.28 ( $\text{CH}_3$ ).

Elemental analysis: Calculated for  $\text{C}_{31}\text{H}_{44}\text{BrNO}_3$  C, 66.66%, H, 7.94%, N, 2.51%; Found: C, 66.78%, H, 7.85%, N, 2.53%.

## Acknowledgements

The author (S.T. Ha) would like to thank Universiti Tunku Abdul Rahman for the financial support and research facilities.

## References and Notes

1. Hadjoudis, E.; Vittarakis, M. Moustakali-Mavridis, I. Photochromism and thermochromism of schiff bases in the solid state and in rigid glasses. *Tetrahedron* **1987**, *43*, 1345-1360.
2. Hadjoudis, E.; Rontogianni, A.; Ambroziak, K.; Dziembowska, T.; Mavridis, I.M. Photochromism and thermochromism of solid trans-N,N'-bis(salicylidene)-1,2-cyclohexanediamines and *trans*-N,N'-bis-(2-hydroxynaphthalene)-1,2-cyclohexanediamine. *J. Photochem. Photobiol. A - Chem.* **2004**, *162*, 521-530.

3. Oshima, A.; Momotake, A.; Arai, T. Photochromism, thermochromism, and solvatochromism of naphthalene-based analogues of salicylideneaniline in solution. *J. Photochem. Photobiol. A - Chem.* **2004**, *162*, 473-479.
4. Yeap, G.Y.; Ha, S.T.; Ishizawa, N.; Suda, K.; Boey, P.L.; Mahmood, W.A.K. Synthesis, crystal structure and spectroscopic study of para substituted 2-hydroxy-3-methoxybenzalideneanilines. *J. Mol. Struct.* **2003**, *658*, 87-99.
5. Yeap, G.Y.; Ha, S.T.; Lim, P.L.; Boey, P.L.; Ito, M.M.; Sanehisa, S.; Youhei, Y. Synthesis, physical and mesomorphic properties of Schiff's base esters containing ortho-, meta- and para-substituents in benzylidene-4'-alkanoyloxyanilines. *Liq. Cryst.* **2006**, *33*, 205-211.
6. Ha, S.T.; Ong, L.K.; Wong, J.P.W.; Yeap, G.Y.; Lin, H.C.; Ong, S.T.; Koh, T.M. Mesogenic Schiff's base ether with dimethylamino end group. *Phase Transit.* **2009**, *82*, 387-397.
7. Ha, S.T.; Ong L.K.; Ong, S.T.; Yeap, G.Y.; Wong, J.P.W.; Koh, T.M.; Lin, H.C. Synthesis and mesomorphic properties of new Schiff base esters with different alkyl chains. *Chin. Chem. Lett.* **2009**, *20*, 767-770.
8. Ha, S.T.; Ong, S.T.; Chong, Y.T.; Yeap, G.Y. Synthesis of 4-{{(3-chlorophenyl)imino]methyl}-3-hydroxyphenyl myristate. *Molbank* **2009**, *2009*, M629.

© 2010 by the authors; licensee Molecular Diversity Preservation International, Basel, Switzerland. This article is an open-access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/3.0/>).