

Ethyl 1-(4-chlorophenyl)-5,6-dimethyl-7,8a-diphenyl-4,5,6,8a-tetrahydro-1H-[1,2,4] triazolo[4,3-c][1,3]diazine-3-carboxylate

A. Boudina,^{*} A. Baouid and A. Hasnaoui

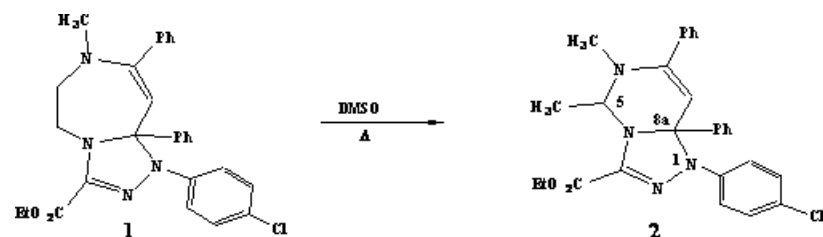
Laboratoire de Chimie des Substances Naturelles et des Hétérocycles, Faculté des Sciences-Semlalia, Université Cadi Ayyad, B.P 2390 Marrakech, Maroc.

e-mail: boudina2@yahoo.fr

*Author to whom correspondence should be addressed

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Compound **1** [1] (200 mg, 0.41 mmol) was refluxed in dimethylsulfoxide for 30 minutes. After cooling, the solvent was removed by evaporation under reduced pressure. The residue obtained was purified by chromatography on silica gel column (eluent: hexane/ethyl acetate 90/10), then the isolated product was recrystallized from ethanol to give **2** (130 mg, 65%).

Melting point: 130-132°C (Ethanol).

MS (m/z, %): 487 ([M+H]⁺, 100%).

¹H-NMR (CDCl₃, 250 MHz): δ= 1.11 (d, J = 6.90 Hz, 3H, CH₃-C-5), 1.44 (t, J = 6.90 Hz, 3H, CH₃-CH₂-O), 2.58 (s, 3H, N-CH₃), 4.41 (q, J = 6.90 Hz, 2H, CH₃-CH₂-O), 5.63 (s, 1H, H-C-8), 5.65 (q, J = 6.90 Hz, 1H, H-C-5), 6.80-7.70 (m, 14H, Ar-H).

¹³C-NMR and DEPT (CDCl₃, 62.5 MHz): δ= 14.21, 19.07 (CH₃-CH₂-O, CH₃-C-5), 41.59 (N-CH₃), 61.86 (CH₃-CH₂-O), 68.13 (C-5), 85.60 (C-8a), 101.33 (C-8).

References:

- Baouid, A.; Benharref, A.; Hasnaoui, A.; Laverge, J.-P. *Bull. Soc. Chim. Belg.* **1994**, *103* (12), 743.

Sample Availability: Available from MDPI.

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