Molecules **1998**, *3*, M52

Ethyl *(Z)*-3-Methyl-5-phenyl-2-pentenoate

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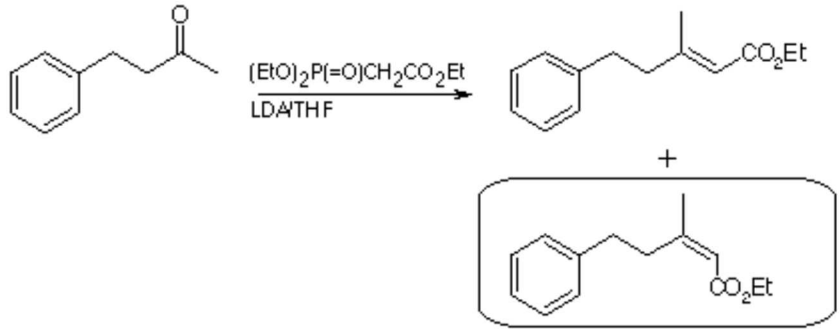
Received: 27 February 1998 / Published: 6 March 1998



The synthetic procedure [1] has been presented elsewhere. Ethyl (*Z*)-3-methyl-5-phenyl-2-pentenoate was obtained (2.23 g, 23%) as a colourless oil.

B.p. 105°/0.5 mmHg (Kugelrohr)

Anal. calc. for $C_{14}H_{18}O_2$ (218.29): C 77.0, H 8.3; found: C 76.9, H 8.1.

UV (ethanol) 310 (289), 210 (16220) nm.

IR (film) 1713 (s, C=O), 1650, 1229, 1165.1053 cm^{-1}

^{1}H-NMR (400 MHz, $CDCl_3$) 1.28 (3H, t, *J* 7.2 Hz, -OCH_2CH_3), 1.88 (3H, d, *J* 1.5 Hz, CH_3), 2.78 (2H, bt, *J* 8.0 Hz, Ph-CH_2), 2.92 (2H, m, CH_2), 4.14 (2H, q, *J* 7.2 Hz, -OCH_2CH_3), 5.69 (1H, tq, *J* 1.1, 1.5 Hz, =CH), 7.16-7.32 (5H, m, ArH). Stereochemistry confirmed by n.O.e. difference spectroscopy. Irradiation at 1.88 produced a 6% n.O.e. at 5.69 (also 1% at 2.92, 1% at 2.78). Irradiation at 5.69 produced an 8% n.O.e. at 1.88.

^{13}C-NMR (15 MHz, $CDCl_3$) 14.15, 25.06 (CH_3), 34.41, 35.32, 59.15, (CH_2), 116.6 (=CH); 125.7, 128.1, 128.1 (CH), 141.5 (quat, C1'), 158.8 (quat, C3), 165.8 (quat, C1).

EI-MS 218 (M^+, 18%), 173(22), 172(12), 145(17), 144(28), 129(!3), 92(13), 91(100), 65(14).

Acknowledgment: The authors gratefully acknowledge financial support from the Australian Research Council and The University of Sydney.

References and Notes

1. Preceding article.

Sample Availability: No sample available.