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

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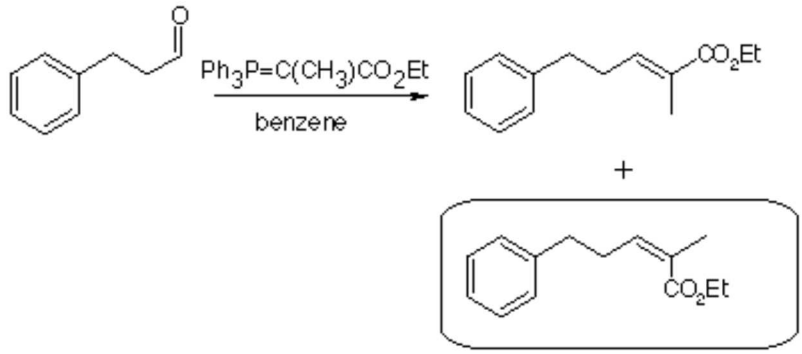

The synthetic procedure [1] has been presented elsewhere. Ethyl (*Z*)-2-methyl-5-phenyl-2-pentenoate (0.24 g, 7%) was prepared as a colourless oil.

B.p. 130°/0.4 mmHg (Kugelrohr)

Anal. calc. for $C_{14}H_{18}O_2$ (218.29): C 77.0, H 8.3; found: C 77.4, H 8.2.

IR (film) 2961, 2928, 1701 (s, C=O), 1456, 1240, 1216, 1184(s), 1124(s), 1030 69(s) cm^{-1}

^{1}H-NMR (400 MHz, $CDCl_3$) 1.29 (3H, t, *J* 7.1 Hz, -OCH_2CH_3), 1.88 (3H, dt, *J* 1.5, 1.2 Hz, CH_3), 2.68-2.82 (4H, m, 2xCH_2), 4.18 (2H, q, *J* 7.1 Hz, -OCH_2CH_3), 5.95 (1H, tq, *J* 7.10, 1.5 Hz, =CH), 7.14-7.32 (5H, m, ArH). Stereochemistry confirmed by n.O.e. difference spectroscopy. Irradiation at 1.88 produced a 16% n.O.e. at 5.95 and irradiation at 5.95 produced a 10% n.O.e. at 1.88.

^{13}C-NMR (15 MHz, $CDCl_3$) 14.02, 20.06 (CH_3), 30.84, 35.32, 59.67, (CH_2), 125.6 (CH), 17.7 (quat, C2), 128.0 (2xCH), 141.0 (=CH); 141.3 (quat, C1'), 167.5 (quat, C1).

EI-MS 218(M^+, 45%), 173(23), 172(15), 144(10), 92(23), 91(100), 65(16).

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References and Notes

1. Preceding article.

Sample Availability: No sample available.