Molecules **1998**, *3*, M73

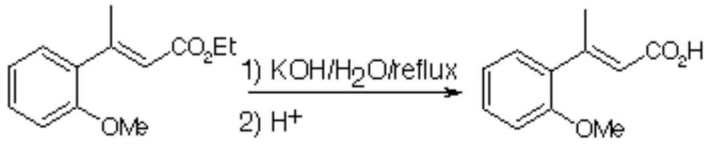
(*E*)-3-(2-Methoxyphenyl)-2-butenoic Acid

Martin J. Stoermer* and John T. Pinhey

Division of Organic Chemistry, School of Chemistry F11, The University of Sydney, N.S.W 2006, Australia.

*Current address: Victorian College of Pharmacy, Monash University (Parkville Campus), 381 Royal Parade, Parkville, Victoria 3052, Australia. Phone: +61 3 990 39000, Fax: +61 3 99039582, e-mail: martin.stoermer@vcp.monash.edu.au, http://synapse.vcp.monash.edu.au/martin/

Received: 27 February 1998 / Published: 6 March 1998



The general part of the experimental section [1] has been presented elsewhere. Ethyl (*E*)-3-(2-methoxyphenyl)-2-butenoate (2.70 g, 12.3 mmol) was refluxed with potassium hydroxide (1.72 g, 30.7 mmol) in a mixture of water (20 ml) and methanol (10 ml) for 3 hours, cooled and washed with ether (100 ml). The aqueous phase was acidified with concentrated hydrochloric acid to below pH 1. The mixture was extracted with ether (100 ml) and the ether extract was washed with water (2x100 ml), brine (50 ml), dried (Na_2SO_4), filtered and evaporated under reduced pressure. (*E*)-3-(2-Methoxyphenyl)-2-butenoic acid (2.14 g, 91%) was obtained as a colourless prisms from ether/light petroleum.

M.p. 102° (lit.[2] (E) and (Z)-mixture, 98°)

UV (ethanol) 285sh (4605), 258 (7748), 216 (18980) nm.

IR ($CDCl_3$) 3300-2800(bs, OH), 1692 (s, C=O), 1631, 1490, 1464, 1436, 1295, 1266, 1239, 1028 cm^{-1}.

^{1}H-NMR (400 MHz, $CDCl_3$) 2.51 (3H, d, *J* 1.5 Hz, CH_3), 3.83 (3H, s, OCH_3), 5.94 (1H, q, *J* 1.5 Hz, =CH), 6.90 (1H, dd, *J* 8.3 1.1 Hz, H3'), 6.95 (1H, ddd, *J* 7.5, 7.4, 1.1 Hz, H5'), 7.16 (1H, dd, *J* 7.5, 1.9 Hz, H6'), 7.31 (1H, ddd, *J* 8.3, 7.4, 1.9 Hz, H4'). Stereochemistry confirmed by n.O.e. difference spectroscopy. Irradiation at 2.51 produced no n.O.e. at 5.94. Irradiation at 5.94 produced no n.O.e. at 2.51 (5% at 7.16).

^{13}C-NMR (15 MHz, $CDCl_3$) 20.13, 55.32 (CH_3), 111.0 (=CH); 118.6, 120.5, 128.6, 129.6 (CH), 132.8 (quat, C1'), 156.2, 159.4(quat), 172.3 (quat, C1).

EI-MS 193(M^++1, 10%), 192(M^+, 56%), 175(24), 166(17), 165(100), 163(27), 145(20), 133(29), 132(27), 131(61), 115(22), 105(39), 103(22), 91(23), 77(29).

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

References and Notes

1. Moloney, M.G.; Pinhey, J.T.; Stoermer, M.J. "Vinyl Cation Formation by Decomposition of Vinyl-lead Triacetates. The reactions of Vinylmercury and Vinyltin Compounds with Lead Tetraacetate." *J. Chem. Soc. Perkin Trans. 1* **1990**, *10*, 2645.

2. Scmitt, J. Suquet, M.; Comoy, P.; Boitard, J.; Callet, G.; Clim, T.; Le Meur, J. *Bull. Soc. Chim. Fr*. **1966**, *3*, 953.

Sample Availability: No sample available.