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3-Hydroxy-3-methyl-5-phenylpentanoic Acid

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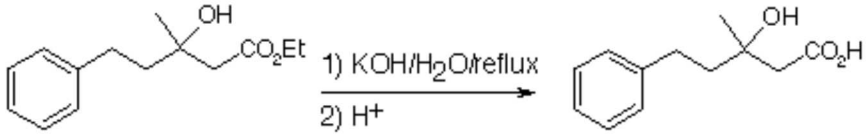

The general part of the experimental section [1] has been presented elsewhere. Ethyl 3-hydroxy-3-methyl-5-phenylpentanoate (1.00 g, 4 mmol) and potassium hydroxide (0.6 g, 11 mmol) in water (20 ml) and methanol (4 ml) were refluxed for 3 hours, cooled and washed with ether (20 ml). The aqueous phase was acidified with concentrated hydrochloric acid to below pH 1 and extracted with ether (3x20 ml). The combined ether extracts were dried (Na_2SO_4), filtered and evaporated under reduced pressure to yield 3-hydroxy-3-methyl-5-phenylpentanoic acid.

(0.57 g, 65%).

M.p. 45°

UV (ethanol) 295 (83), 268 (223), 261 (285), 255sh (250), 249 (202) nm.

IR ($CDCl_3$) 3500-2800(bs, OH), 3029, 2982, 1707 (s, C=O), 704 cm^{-1}.

^{1}H-NMR (90 MHz, $CDCl_3$) 1.33 (3H, s, CH_3), 1.83 (2H, m, CH_2), 2.55 (2H, s, CH_2), 2.68 (2H, s, Ph-CH_2), 6.92 (2H, bs, 2xOH), 7.12 (5H, m, ArH).

^{13}C-NMR (15 MHz, $CDCl_3$) 26.56 (CH_3), 30.19, 43.63, 44.74 (CH_2), 71.36 (quat, C3), 125.8, 128.2 128.4 (ArCH), 141.8 (quat, C1'), 177.1 (quat, C1).

EI-MS 190(M^+-H_2O, 31%), 131(63), 105(25), 103(18), 91(100), 85(12).

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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.

Sample Availability: No sample available.