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1-Ethyl 4-(2-oxopropyl) 2-(1,2,3,4-Tetrahydro-1,3-dimethyl-2,4-dioxopyrimidin-5-yl)butanedioate

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Scheme

The diester **2** was prepared by the addition of 2-hydroxyacetone to **1** according to the reported procedure [1].

2-Hydroxyacetone (0.2 ml, 2.9 mmol) was added to a solution of **1** (293 mg, 1 mmol) in CH₂Cl₂ (5 ml). The mixture was left at r.t. for 2 h and filtered through a pad of silica gel (EtOAc) afforded the title compound **2**, a colourless oil: 320 mg (94 %).

IR (neat): 3070m, 1725vs, 1700vs, 1660vs, 1640vs, 1483s, 1460s, 1435s, 1375s, 1350s, 1275s, 1250s, 1190s, 1155s, 1090s, 1020s, 780s, 755s.

¹H-NMR (CDCl₃): 7.30 (s, 1H, H-6'); 5.66 (s, 2H, CO₂C H_2 COCH₃); 4.16 (q, J = 7.1, 2H, CO₂C H_2 Me), 3.88 (dd, J = 8.2, 5.7, H-2); 3.41 (s, Me-1'); 3.32 (s, Me-3'); 3.18 (dd, J = 16.8, 5.7, 1H, H-3); 2.92 (dd, J = 16.8, 8.2, 1H, H-3); 2.13 (s, 3H, CO₂CH₂COC H_3); 1.23 (t, J = 7.1, CO₂CH₂C H_3).

¹³C-NMR (CDCl₃): 207.5 (CO₂CH₂COCH₃), 173.4 (CO₂CH₂COCH₃), 171.3 (CO₂CH₂Me), 162.0 (C-4'), 151.0 (C-2'), 141.7 (C-6'), 109.7 (C-5'), 67.9 (CO₂CH₂COCH₃), 60.8 (CO₂CH₂Me), 39.5 (C-2), 36.5 (Me-3'), 34.2 (C-3), 27.3 (Me-1'), 24.7 (CO₂CH₂COCH₃), (CO₂C(CH₃)₃), 13.4 (CO₂CH₂CH₃).

EI-MS: 340 (M⁺, 4), 295 (4), 294 (10), 267 (5), 266 (13), 239 (2), 238 (8), 237 (6), 194 (12), 193 (100), 169 (2), 167 (5), 166 (13), 165 (11), 110 (2), 81 (15), 80 (8), 69 (2), 68 (4), 56 (2).

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References

1. Zhuo, J.-C.; Wyler, H. Helv. Chim. Acta 1993, 76, 1916.

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