

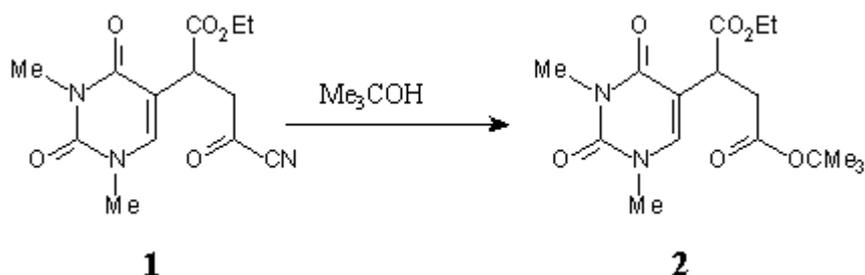
Molecules **1997**, *2*, M8

1-Ethyl 4-(1,1-dimethylethyl) 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 tert-butanol to **1** according to the reported procedure [1].

tert-Butanol (0.2 ml) was added to a solution of **1** (293 mg, 1 mmol) in CH₂Cl₂ (5 ml). The mixture was left at r.t. for 3 h. Evaporation of the solvent under reduced pressure afforded the title compound **2**, a colourless oil: 340 mg (100 %).

IR (neat): 3070m, 1730vs, 1705vs, 1660vs, 1645vs, 1480s, 1460s, 1365s, 1345s, 1275s, 1255s, 1180s, 1150s, 1020s, 845s, 780s, 755s.

¹H-NMR (CDCl₃): 7.23 (s, 1H, H-6'); 4.20 and 4.15 (2x dq, J = 11.0, 7.1, CO₂CH₂Me), 3.90 (dd, J = 7.1, 6.7, H-2); 3.39 (s, Me-1'); 3.34 (s, Me-3'); 2.95 (dd, J = 16.8, 6.7, 1H, H-3); 2.67 (dd, J = 16.8, 7.1, 1H, H-3); 1.41 (s, 9H, CO₂C(CH₃)₃); 1.24 (t, J = 7.1, CO₂CH₂CH₃).

¹³C-NMR (CDCl₃): 173.6 (CO₂C(CH₃)₃), 171.5 (CO₂CH₂Me), 162.2 (C-4'), 151.1 (C-2'), 141.7 (C-6'), 110.0 (C-5'), 69.1 (CO₂C(CH₃)₃), 61.0 (CO₂CH₂Me), 39.7 (C-2), 36.7 (Me-3'), 34.6 (C-3), 27.6 (Me-1'), 30.5 (CO₂C(CH₃)₃), 13.6 (CO₂CH₂CH₃).

EI-MS: 340 (M⁺, 1), 285 (4), 284 (28), 267 (17), 266 (5), 239 (21), 238 (52), 237 (4), 210 (23), 194 (11), 193 (90), 169 (8), 167 (35), 166 (49), 165 (24), 110 (10), 81 (33), 80 (18), 69 (3), 68 (8), 59 (14), 58 (12), 57 (100), 56 (11).

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References

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

Sample Availability: Available from MDPI, 0.3g, MDPI 10058.

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