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1,5-Bis(4-methylphenyl)-3-phenylpentane-1,5-dione

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The title compound, $C_{25}H_{24}O_2$, has been synthesized by the reaction of benzaldehyde with 4-methylacetophenone and NaOH. The bond lengths and angles show normal values. The crystal packing exhibits no significantly short intermolecular contacts.

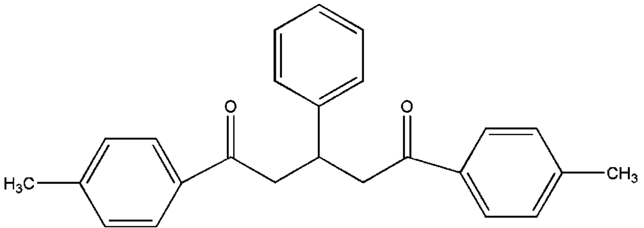
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.042
wR factor = 0.126
Data-to-parameter ratio = 8.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Recently, solvent-free organic reactions (Toda, 1995; Loupy, 2000; Cave *et al.*, 2001) have attracted great attention due to the increasing concern for the protection of the environment (DeSimone, 2002; Tanaka, 2003; Tanaka & Toda, 2000; Metzger, 1998). 1,5-Diketones are important synthetic intermediates and starting materials in the synthesis of many heterocyclic compounds (Hirsch & Bailey, 1978; Krohnke, 1976). In a continuation of previous work on the synthesis of 1,5-diketones (Constable *et al.*, 1998; Fuchigami *et al.*, 1986), we present a new compound, 1,5-bis(4-methylphenyl)-3-phenylpentane-1,5-dione, (I), synthesized under solvent-free conditions.



(I)

In the molecule (Fig. 1), the bond lengths and angles are normal and correspond to those observed in 1,3,5-triphenylpentane-1,5-dione (Das *et al.*, 1994). The crystal packing demonstrates no significantly short intermolecular contacts.

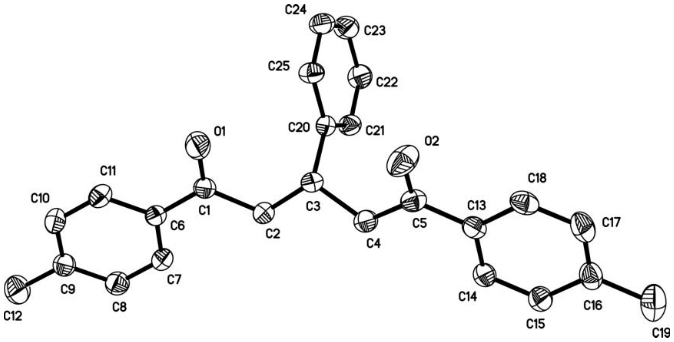


Figure 1
View of (I) with the atomic numbering and displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

Experimental

4-Methylacetophenone (0.75 g, 6.25 mmol), freshly distilled benzaldehyde (0.33 g, 3.125 mmol) and NaOH (0.25 g, 6.25 mmol) were aggregated with a glass paddle in an open flask. The resulting mixture was washed with water several times to remove NaOH and was recrystallized from ethanol, affording the title compound as a crystalline solid.

Crystal data

$C_{25}H_{24}O_2$
$M_r = 356.44$
Orthorhombic, $P2_12_12_1$
$a = 5.715$ (3) Å
$b = 15.848$ (8) Å
$c = 21.386$ (11) Å
$V = 1936.8$ (17) Å^3
$Z = 4$
$D_x = 1.222$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.23 × 0.18 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.983$, $T_{\max} = 0.989$
10270 measured reflections
1998 independent reflections
1166 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.076$
$\theta_{\max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.126$
$S = 1.01$
1998 reflections
244 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.056P)^2 + 0.0975P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.15$ e Å^{-3}
$\Delta\rho_{\min} = -0.15$ e Å^{-3}

All H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined as riding, with $U_{\rm iso}$(H) = $U_{\rm eq}$(C). Due to the absence of any significant anomalous scatterers in the molecule, the 1409 Friedel pairs were merged before the final refinement.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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