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

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.164
Data-to-parameter ratio = 13.8

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

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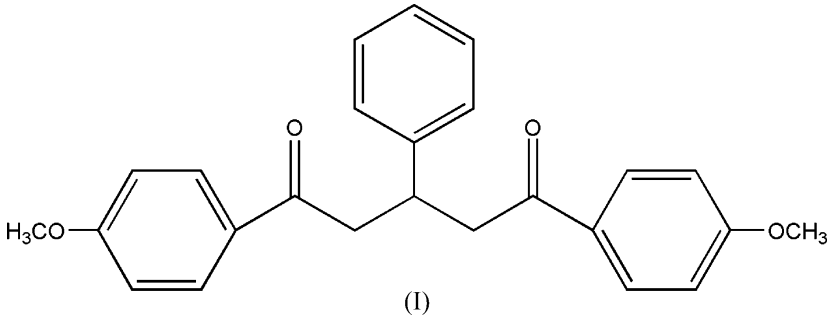
In the title molecule, $C_{25}H_{24}O_4$, the central phenyl ring makes dihedral angles of 85.92 (12) and 78.21 (13)° with the two outer benzene rings. The crystal packing is stabilized by van der Waals forces.

Comment

In a continuation of our ongoing program directed to the development of environmentally benign methods of chemical synthesis (Hajipour *et al.*, 2004, 2005), we present here the crystal and molecular structure of the title compound, (I), which was synthesized in the presence of KOH under solvent-free conditions.



(I)

In (I) (Fig. 1), all bond lengths and angles are normal and agree with those observed in 1,3,5-triphenyl-pentane-1,5-diketone (Das *et al.*, 1994) and 1,5-diphenyl-3-(2-pyridyl)-pentane-1,5-dione (Huang *et al.*, 2006). The aromatic rings C20–C25 (*A*), C2–C7 (*B*) and C10–C15 (*C*) make dihedral angles *A*/*B*, *A*/*C* and *B*/*C* of 85.92 (12), 78.21 (13) and 9.5 (2)°, respectively. The crystal packing is stabilized by van der Waals forces.

Experimental

4-Methoxyacetophenone (0.94 g, 6.25 mmol), freshly distilled benzaldehyde (0.33 g, 3.125 mmol) and KOH (0.35 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 KOH, and recrystallized from ethanol to afford the title compound.

Crystal data

$C_{25}H_{24}O_4$
M_r = 388.44
Monoclinic, $P2_1/n$
a = 5.673 (3) Å
b = 24.014 (14) Å
c = 15.059 (9) Å
β = 94.028 (9)°
V = 2046 (2) Å^3
Z = 4
D_x = 1.261 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, colourless
0.35 × 0.17 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer	10442 measured reflections
φ and ω scans	3607 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	1599 reflections with $I > 2\sigma(I)$
$T_{min} = 0.971$, $T_{max} = 0.987$	$R_{int} = 0.065$
	$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.051$	$w = 1/[\sigma^2(F_o^2) + 0.4792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.164$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
3607 reflections	$\Delta\rho_{min} = -0.16$ e Å^{-3}
262 parameters	

All H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.98 Å and U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; 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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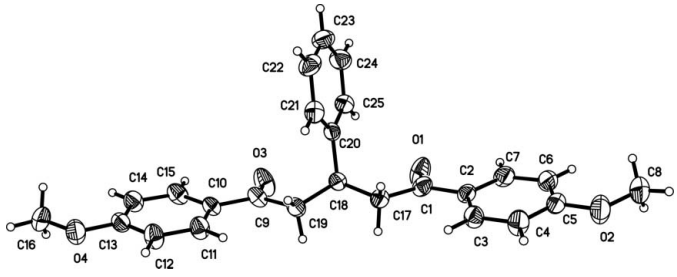

Figure 1
The molecular structure of (I) with the atom-numbering scheme and 30% probability displacement ellipsoids.

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