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(*E*)-3-(1,3-Benzodioxol-5-yl)-1-phenyl-2-propen-1-one

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In the title compound, $C_{16}H_{12}O_3$, the dihedral angle between the benzene rings is 12.0 (1)°. In the crystal structure, the molecules are linked through π–π interactions and C–H···π (arene) hydrogen-bonding interactions.

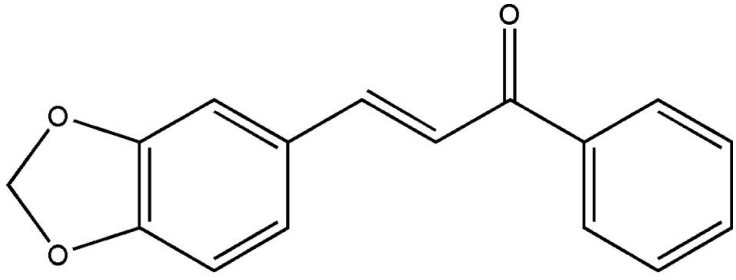
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.002 Å
R factor = 0.047
wR factor = 0.110
Data-to-parameter ratio = 13.9

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

Comment

Chalcones are important biological compounds. They show antibacterial, antifungal, antitumor and anti-inflammatory properties (Dimmock *et al.*, 1999). They are also intermediates in the biosynthesis of flavonoids, which are substances widespread in plants and with an array of biological activities (Le Bail *et al.*, 2001). The title compound, (I), was synthesized by AlvarezIbarra *et al.* (1992). However, we have recently reexamined (I) and its structure is reported here.



(I)

In the molecular structure of (I) (Fig. 1), the C1–C6 phenyl ring is taken as plane 1, C10–C15 as plane 2, and the central atoms, C7–C10, as plane 3, with dihedral angles between them, A_{12}, A_{13} and A_{23} of 12.0 (1), 24.0 (1) and 15.1 (1)°, respectively, showing that the two benzene rings are rotated in opposite directions with respect to plane 3. The torsion angle C7—C8—C9—C10 is −177.7 (17)° and keto atom O1 deviates from plane 3 by 0.23 (1) Å. The dioxylmethylene group attached at C13 and C14 is slightly twisted with respect to plane 2, with torsion angles C14—C13—O3—C16 and C13—C14—O2—C16 of 5.1 (2) and −4.5 (2)°, respectively.

In the crystal structure, molecules are paired by C—H···π(arene) interactions *via* H12 to the centroid of C10–C15, *Cg*, in an adjacent molecule (symmetry code: $\frac{1}{2} - x, \frac{1}{2} + y, z$). Furthermore, weak π–π stacking intermolecular interactions are present, such that the benzene rings (C1–C6) belonging to adjacent layers form pairs of molecules related by centers of symmetry. The centroid–centroid distance involved is 3.993 (1) Å and the perpendicular distance is 3.55 (1) Å, with the benzene rings in adjacent layers lying parallel to each other (Fig. 2).

Experimental

The title compound was synthesized by grinding a mixture of acetophenone (6.01 g, 0.05 mol), 3,4-dioxymethylenebenzaldehyde (7.51 g, 0.05 mol), NaOH (0.2 g, 0.005 mol) and K_2CO_3 (3.46 g, 0.025 mol) at room temperature for 20 min. The resulting solid was washed with water until neutral. The residue was recrystallized from ethanol (yield 90%). Crystals suitable for X-ray analysis were obtained at room temperature by slow evaporation of a dichloromethane and petroleum ether (1:1 *v*/*v*) solution (m.p. 380–382 K).

Crystal data

$C_{16}H_{12}O_3$
M_r = 252.26
Orthorhombic, *Pbca*
a = 11.4464 (11) Å
b = 7.5202 (7) Å
c = 28.277 (3) Å
V = 2434.1 (4) Å^3
Z = 8
D_x = 1.377 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 292 (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2001)
T_{min} = 0.972, T_{max} = 0.981
13993 measured reflections
2388 independent reflections
1817 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.110
S = 1.07
2388 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.5194P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···Cg^{i}	0.93	2.95	3.810 (2)	155

Symmetry code: (i) $x, -y-\frac{1}{2}, z-\frac{1}{2}$. *Cg* is the centroid of atoms C10–C15.

All H atoms were placed in calculated positions and refined using the riding model (C—H = 0.93–0.97 Å), with U_{iso}(H) 1.2U_{eq}(C).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

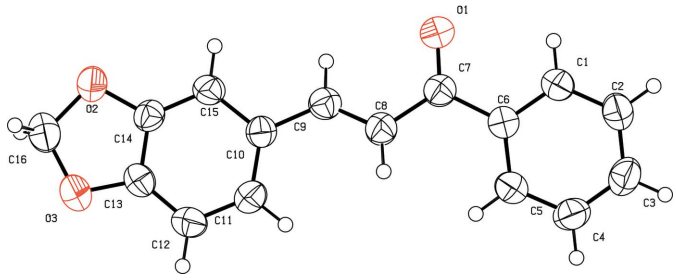


Figure 1
The molecular structure and atom-labelling scheme of (I). Displacement ellipsoids are drawn at the 50% probability level.

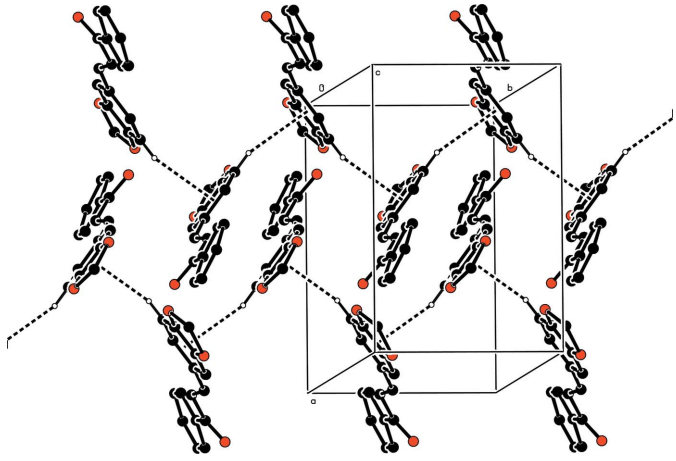


Figure 2
Packing diagram showing the crystal structure of the title compound, (I), in the *ab* plane. C—H···π interactions are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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