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3-(1,3-Benzodioxol-5-yl)-1-phenylprop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.001 Å
R factor = 0.034
wR factor = 0.092
Data-to-parameter ratio = 16.3

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

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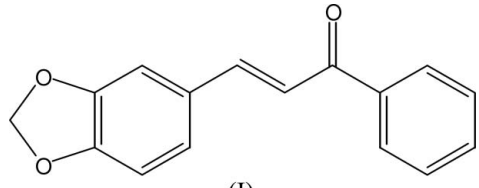
In the title biologically active compound, $C_{16}H_{12}O_3$, the central C=C double bond is *trans* configured. The molecule consists of two essentially planar parts which are twisted by 26.89 (5)° with respect to each other.

Comment

Chalcones possess a broad spectrum of biological activities, including antibacterial, antihelmintic, amoebicidal, anti-ulcer, antiviral, insecticidal, antiprotzoal, anticancer, cytotoxic and immunosuppressive activities (Dimmock *et al.*, 1999). Certain chalcone derivatives were reported to inhibit the polymerization of tubulin to form microtubules and were therefore antimitotic agents which can be used as anti-inflammatory agents. Chalcone derivatives were also reported to inhibit the destruction of myelin sheath in the central nervous system of multiple sclerosis patients and were thus useful in controlling the progressive nature of the disease (Edwards *et al.*, 1989). Chalcones can be easily obtained from the aldol condensation of aromatic aldehydes and aromatic ketones. This class of compounds presents interesting biological properties, such as cytotoxicity (Lawrence *et al.*, 2001), antiherpes activity and antitumour activity and may be useful for the chemotherapy of leishmaniasis (Pandey *et al.*, 2005), among others. A comparison of the supramolecular structures of 1-(6-amino-1,3-benzodioxol-5-yl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one and 1-(6-amino-1,3-benzodioxol-5-yl)-3-[4-(*N*,*N*-dimethylamino)phenyl]prop-2-en-1-one has been described previously (Low *et al.*, 2002). The crystal structure of (1,3-benzodioxol-5-ylmethyl)ammonium 2-methoxy-5-[(1*E*)-3-oxo-3-phenylprop-1-en-1-yl]benzenesulfonate monohydrate (da Silva *et al.*, 2006) has recently been reported. In view of the importance of the title compound, (I), its crystal structure is reported here.



(I)

The molecular structure of the title compound is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Crystallographic Database, Version 5.27, November 2005 updated May 2006; Mogul Version 1.1; Allen, 2002). The central C=C double bond is *trans* configured. The molecule consists of two planar segments which are twisted by 26.89 (5)° with respect to each other. One of these contains the

1,2-(methylenedioxy)benzene group which is coplanar with the propenone group (r.m.s. deviation for all non H atoms 0.049 Å), and the other segment is the phenyl ring. All torsion angles are close to 0 or 180°; only those about the C10—C11 bond differ significantly from planarity (Table 1). The crystal packing shows a herringbone pattern (Fig. 2) and reveals one weak C—H···O contact (Table 2).

Experimental

The title compound was synthesized according to the method reported in the literature (Vogel, 1989) with a yield of 75%. The compound was purified by recrystallization from ethanol. The crystal growth was performed in acetone solvent by slow evaporation (m.p. 365 K). Analysis found (calculated) for $C_{16}H_{12}O_3$: C 76.20 (76.18), H 4.75 (4.79)%.

Crystal data

$C_{16}H_{12}O_3$
M_r = 252.26
Orthorhombic, *Pbca*
a = 11.1234 (5) Å
b = 7.7504 (4) Å
c = 28.4607 (11) Å
V = 2453.62 (19) Å^3
Z = 8
D_x = 1.366 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 173 (2) K
Plate, light yellow
0.38 × 0.21 × 0.19 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: none
31874 measured reflections
2813 independent reflections
2590 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.092
S = 1.04
2813 reflections
173 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.6049P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.033 (2)

Table 1
Selected torsion angles (°).

C6—C8—C9—C10	−178.11 (9)	O10—C10—C11—C12	−25.96 (14)
O10—C10—C11—C16	151.40 (11)	C9—C10—C11—C12	154.85 (9)
C9—C10—C11—C16	−27.79 (14)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O10^{i}	0.99	2.59	3.0397 (14)	107

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, -z+1$.

H atoms were found in a difference map, but placed geometrically and allowed to ride on their parent C atoms at distances of 0.95 and 0.99 Å for aromatic and methylene groups, respectively, and with U_{iso}(H) = 1.2U_{eq}(C).

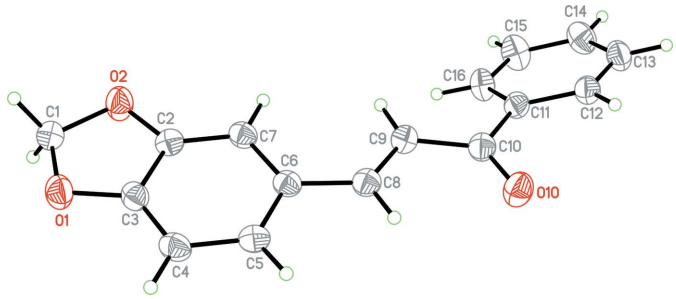


Figure 1
The molecular structure of (I), with the atom numbering; displacement ellipsoids are at the 50% probability level.

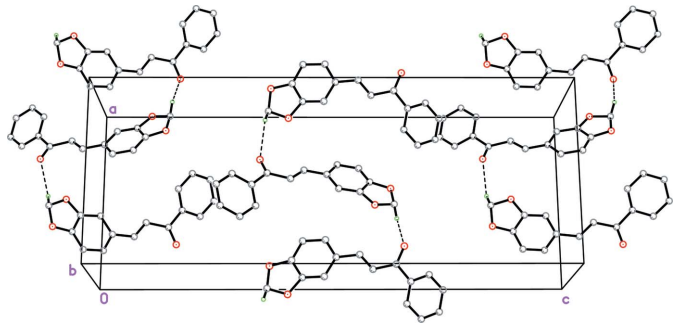


Figure 2
Packing diagram of the title compound, with a view approximately along the b axis. Weak C—H···O hydrogen bonds are shown as dashed lines, and H atoms not involved in these interactions have been omitted.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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