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

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, antiprotozoal, 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), antiviral 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-[(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-[(1E)-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.
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 C16H12O3: C 76.20 (76.18), H 6.72 (6.73), O 17.08 (17.13). 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 C16H12O3: C 76.00 (76.18), H 6.72 (6.73), O 17.28 (17.13).

Crystal data
C16H12O3
M, = 252.26
Orthorhombic, Pbca
a = 11.1234 (5) Å
b = 7.7504 (4) Å
c = 28.4607 (11) Å
V = 2453.62 (19) Å³
Z = 8
D, = 1.366 Mg m⁻³
Mo Kα 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
ø scans
Absorption correction: none
2813 independent reflections
31874 measured reflections
Refinement
Refinement on F²
wR(F²) = 0.092
S = 1.04
2590 reflections with I > 2σ(I)
θmax = 27.6°

Table 1
Selected torsion angles (°).

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<td>−178.11 (9)</td>
<td>−25.96 (14)</td>
<td>154.85 (9)</td>
<td>151.40 (11)</td>
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Table 2
Hydrogen-bond geometry (Å, °).

D—H···A          D—H   H···A       D···A     D—H···A
Cl1—H1A···O10    0.99  2.59  3.0397 (14)  107°

Symmetry code: (i) x−1/2, −y+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(eq)(H) = 1.2Ueq(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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References