1-(2,4-Dichlorophenyl)-3-(4-methoxyphenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study

T = 100 K

Mean σ(C–C) = 0.002 Å

R factor = 0.037

wR factor = 0.113

Data-to-parameter ratio = 32.9

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

In the title compound, $C_{16}H_{12}Cl_2O_2$, the dihedral angle between the benzene rings is 44.59 (3)°. In the crystal structure, the molecules form layers parallel to the *ac* plane which propagate down the *b* axis and which are stabilized by short Cl···Cl interactions.

Comment

Numerous studies dealing with flavonoids, and chalcones in particular, have been carried out in the past few years. The interest in these substances for several disciplines lies in their photochemical behaviour (Matsushima & Kageyama, 1985; Toda *et al.*, 1998), their structural features (Teh *et al.*, 2006; Ng *et al.*, 2006; Patil *et al.*, 2006), and their second-order non-linear optical (NLO) properties (Fichou *et al.*, 1988; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006). In view of these features, we report here the structure of the chalcone derivative, (I) (Fig. 1).
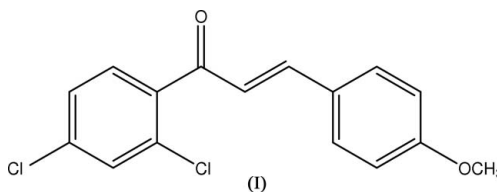
The bond lengths and angles in (I) have normal values (Allen *et al.*, 1987), which are comparable to those in related structures (Ng *et al.*, 2006; Patil *et al.*, 2006; Rosli *et al.*, 2006; Teh *et al.*, 2006). The dihedral angle between the two benzene rings is 44.59 (3)°. The least-squares plane through the O1/C7/C8/C9 enone group makes dihedral angles of 42.89 (4) and 5.85 (4)°, respectively, with the C1–C6 and C10–C15 benzene rings. Atoms Cl1 and Cl2 deviate by 0.0310 (3) and 0.0489 (3) Å, respectively, from the C1–C6 benzene ring. The methoxy group at C13 is almost coplanar with the C10–C15 benzene ring, with a C16—O2—C13—C14 torsion angle of 179.6 (1)°.

Two intramolecular hydrogen bonds are observed in the molecular structure of (I) (Table I). The intramolecular C9—H9A···O1 and C8—H8A···Cl1 interactions generate $S(5)$ and $S(6)$ ring motifs, respectively (Bernstein *et al.*, 1995). The crystal structure consists of layers of molecules, propagating down the *b* axis, stabilized by two short Cl···Cl interactions [3.3913 (4) Å], by which each molecule is linked to others related by the symmetry operations $(1 - x, -\frac{1}{2} + y, \frac{1}{2} - z)$ and $(1 - x, \frac{1}{2} + y, \frac{1}{2} - z)$.

Experimental

Compound (I) was synthesized by the Claisen–Schmidt condensation of 4-methoxybenzaldehyde (0.01 mol) with 2,4-dichloroaceto-
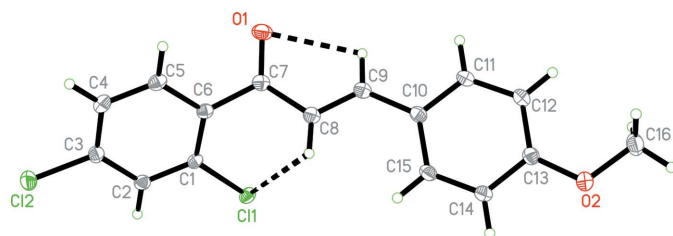
Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Intramolecular hydrogen bonds are drawn as dashed lines.
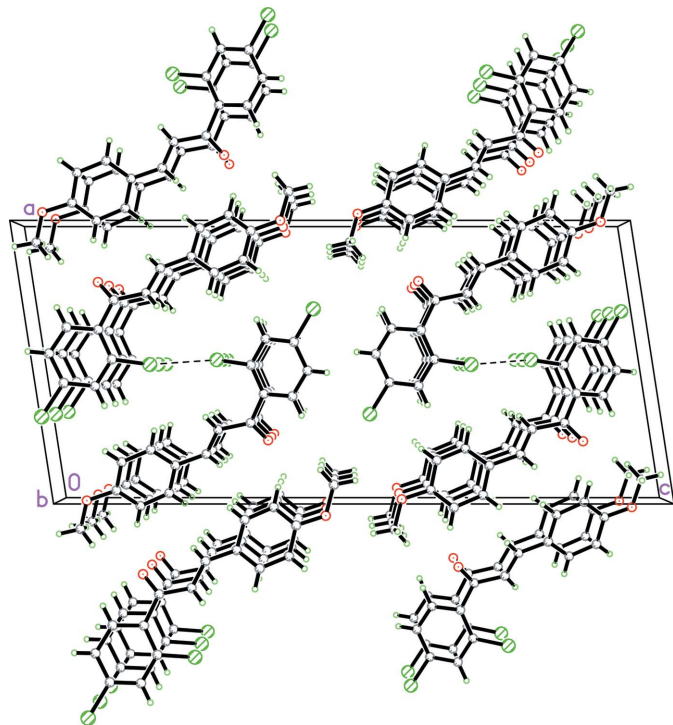

Figure 2
The crystal packing of (I), viewed down the *b* axis. Short Cl···Cl contacts are shown as dashed lines.

phenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (5 ml, 30%). After stirring for 3 h, the contents of the flask were poured into ice-cold water (250 ml), and left to stand for 24 h. The resulting crude solid was collected by filtration, dried and purified by repeated recrystallization from acetone. The purity of the compound was checked by thin-layer chromatography. Crystals suitable for single-crystal X-ray diffraction were grown over a period of 7 days by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{16}H_{12}Cl_2O_2$	$D_x = 1.495$ Mg m^{-3}
$M_r = 307.16$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5994
$a = 12.8259 (2)$ Å	reflections
$b = 3.8806 (1)$ Å	$\theta = 1.5–35.0°$
$c = 27.7348 (4)$ Å	$\mu = 0.47$ mm^{-1}
$\beta = 98.779 (1)°$	$T = 100.0 (1)$ K
$V = 1364.25 (5)$ Å^3	Block, yellow
$Z = 4$	$0.40 \times 0.40 \times 0.22$ mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	5994 independent reflections
ω scans	5307 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$R_{int} = 0.026$
	$\theta_{max} = 35.0°$
$T_{min} = 0.819$, $T_{max} = 0.905$	$h = -19 \rightarrow 20$
25104 measured reflections	$k = -6 \rightarrow 4$
	$l = -44 \rightarrow 44$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0591P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.037$	$+ 0.4152P]$
$wR(F^2) = 0.113$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} = 0.001$
5994 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
182 parameters	$\Delta\rho_{min} = -0.28$ e Å^{-3}
H-atom parameters constrained	

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
C8—H8A···Cl1	0.93	2.79	3.138 (1)	103
C9—H9A···O1	0.93	2.45	2.802 (1)	102

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.96 Å. U_{iso}(H) values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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