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1-(2,4-Dichlorophenyl)-3-(2-furyl)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 = 0.042
wR factor = 0.113
Data-to-parameter ratio = 38.6

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

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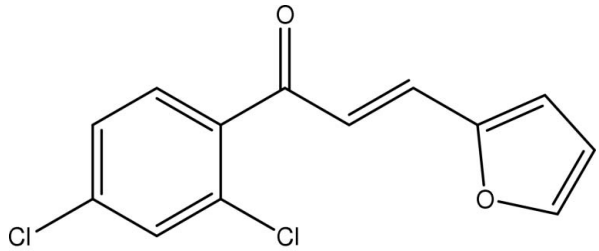
In the title compound, $C_{13}H_8Cl_2O_2$, the dihedral angle between the benzene and furan rings is 44.39 (7)°. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds.

Comment

The title compound, (I), is a derivative of chalcone, 1,3-diphenylprop-2-en-1-one. These compounds display a wide variety of pharmacological effects, including antibacterial, antiviral, antimutagenic, antimitotic, anti-inflammatory, anti-ulcerative and hepatoprotective activities (Batt *et al.*, 1993; Sogawa *et al.*, 1994; Arty *et al.*, 2000). In addition, with appropriate substituents, chalcones are a class of non-linear optical materials (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Uchida *et al.*, 1998; Goto *et al.*, 1991; Patil *et al.*, 2006*a*,*b*; Zhang *et al.*, 1990; Zhao *et al.*, 2000). The single-crystal X-ray structural study of (I) was undertaken in order to establish the structure and conformation of the various groups. Compound (I) does not exhibit second-order non-linear optical properties as it crystallizes in a centrosymmetric space group.



(I)

In (I), bond lengths and angles have normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Ng *et al.*, 2006; Patil *et al.*, 2006, 2006*a*,*b*; Teh *et al.*, 2006). The least-squares plane through the O2/C5/C6/C7 enone group makes dihedral angles of 43.30 (5) and 4.74 (7)° with the C8–C13 (benzene) and C1–C4/O1 (furan) rings, respectively; the dihedral angle between the benzene and furan rings is 44.39 (7)°.

Two intramolecular hydrogen bonds, C5—H5*A*···O2 and C6—H6*A*···Cl1, generate *S*(5) and *S*(6) ring motifs, respectively (Bernstein *et al.*, 1995) (Fig. 1 and Table 1). The molecules form dimers and these dimeric molecules are arranged in layers parallel to the *ac* plane, propagating along the *b* axis. The benzene and furan rings are stacked with a centroid–centroid distance of 3.894 Å, indicating a weak π–π interaction.

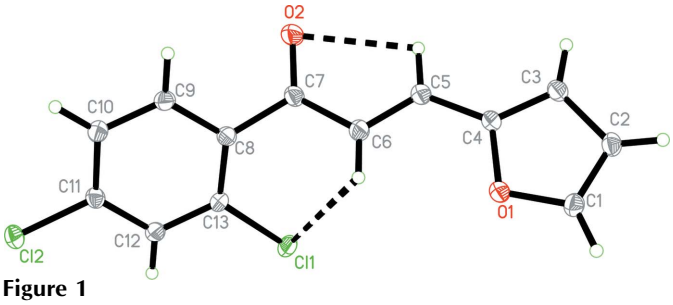


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Dashed lines indicate hydrogen bonds.

Experimental

(I) was prepared *via* condensation of 2-furfuraldehyde (0.01 mol) with 2,4-dichloroacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (5 ml, 25%). After stirring for 2 h, the contents of the flask were poured into ice-cold water (250 ml), and left to stand overnight. The resulting crude solid was collected by filtration, dried and purified by repeated recrystallization from acetone. Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of an acetone solution at room temperature over 7 d.

Crystal data

$C_{13}H_8Cl_2O_2$
M_r = 267.09
Monoclinic, $P2_1/c$
a = 15.5442 (2) Å
b = 3.8939 (1) Å
c = 21.6258 (3) Å
β = 120.330 (1)°
V = 1129.80 (4) Å^3
Z = 4
D_x = 1.570 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.56 mm^{-1}
T = 100.0 (1) K
Block, yellow
0.28 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.832, T_{max} = 0.945
23831 measured reflections
5944 independent reflections
4177 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 37.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.113
S = 1.05
5944 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 0.3596P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5A···O2	0.93	2.46	2.797 (2)	102
C5—H5A···O2^{i}	0.93	2.50	3.308 (2)	146
C6—H6A···Cl1	0.93	2.83	3.194 (2)	105

Symmetry code: (i) $-x+1, -y-1, -z+1$.

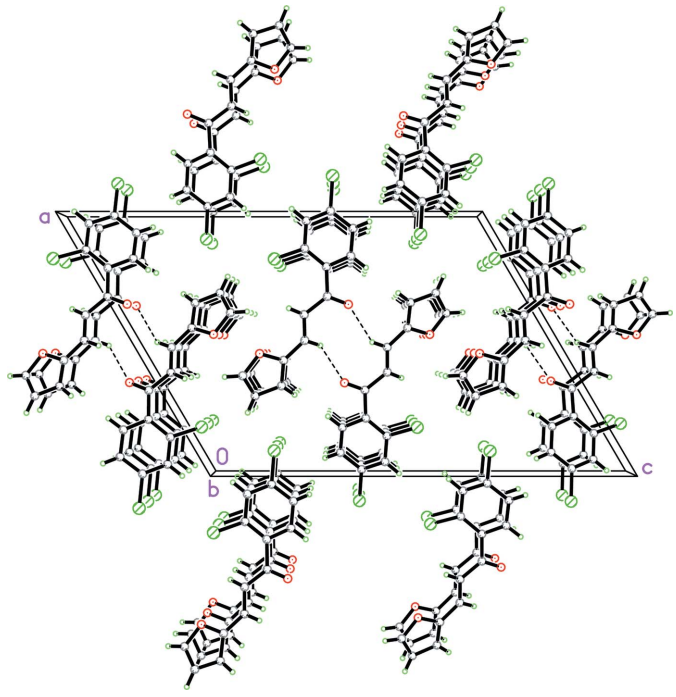


Figure 2
The crystal packing of (I), viewed down the b axis. Intermolecular hydrogen bonds are shown as dashed lines.

All H atoms were refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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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