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# 1-(4-Chlorophenyl)-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 = 0.054
*wR* factor = 0.177
Data-to-parameter ratio = 33.1

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

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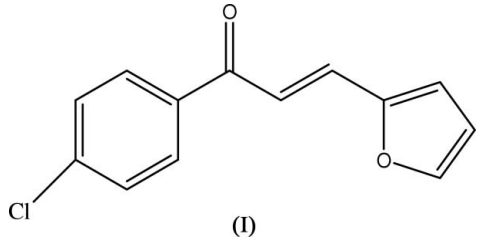
In the title compound, $C_{13}H_9ClO_2$, the dihedral angle between the furan and benzene rings is 44.92 (6)°. The crystal structure is stabilized by C—H···π interactions.

## Comment

Chalcones can be easily obtained from the aldol condensation of aromatic aldehydes and aromatic ketones. This class of compounds presents interesting biological and pharmacological activities (De Vincenzo *et al.*, 1995; Kumar *et al.*, 2003). In addition, chalcone derivatives have attracted much interest as they exhibit extremely high and fast non-linearity (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). We present here a study of molecular packing in the title compound, (I), which crystallizes with a centrosymmetric crystal structure and hence does not exhibit second-order nonlinear optical properties.




(I)

Bond lengths and angles in (I) show normal values (Allen *et al.*, 1987) and are comparable to those observed in related structures (Teh *et al.*, 2006; Patil *et al.*, 2006*a*,*b*; Ng *et al.*, 2006; Rosli *et al.*, 2006). The least-squares plane through the enone group makes dihedral angles of 18.97 (7) and 26.22 (6)° with the C1–C4/O1 and C8–C13 rings, respectively. The dihedral angle between the furan and benzene rings is 44.92 (6)°.

In the molecular structure of (I), the C5—H5*A*···O2 interaction generates an *S*(5) ring motif (Bernstein *et al.*, 1995). The crystal structure is stabilized by C—H···π interactions, involving the C1–C4/O1 ring (Table 1). *Cg*1 is the C1–C4/O1 ring centroid.

## Experimental

The chalcone derivative (I) was obtained by the condensation of 2-furfuraldehyde (0.01 mol) with 4-chloroacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (3 ml, 30%). The mixture was stirred and left standing overnight. 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

experiments were grown in 7 d by slow evaporation of an acetone solution at room temperature.

*Crystal data*

$C_{13}H_9ClO_2$
$M_r$ = 232.65
Monoclinic, $P2_1/c$
$a$ = 13.7630 (2) Å
$b$ = 13.6545 (2) Å
$c$ = 5.7263 (1) Å
$\beta$ = 98.456 (1)°
$V$ = 1064.43 (3) Å$^3$
$Z$ = 4
$D_x$ = 1.452 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.34 mm$^{-1}$
$T$ = 100.0 (1) K
Block, yellow
0.32 × 0.17 × 0.13 mm

*Data collection*

Bruker SMART APEX2 CCD area-detector diffractometer
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min}$ = 0.861, $T_{max}$ = 0.957
20578 measured reflections
4798 independent reflections
3444 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.035
$\theta_{max}$ = 35.3°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.177
$S$ = 1.07
4798 reflections
145 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0886P)^2 + 0.4694P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.98 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.63 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C5—H5$A$···O2 | 0.93 | 2.48 | 2.800 (2) | 100 |
| C12—H12$A$···$Cg1^{i}$ | 0.93 | 2.83 | 3.499 (2) | 130 |

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

H atoms were placed in calculated positions, C—H = 0.93 Å, and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(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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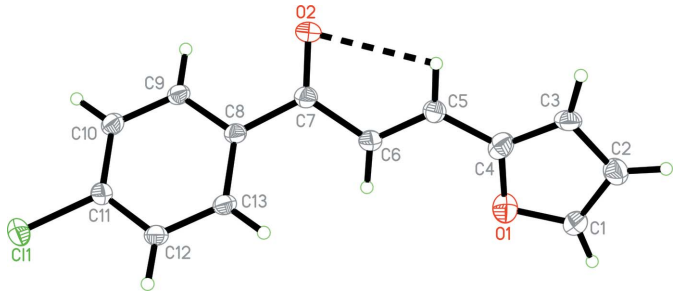


**Figure 1**
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The intramolecular hydrogen bond is drawn as a dashed line.

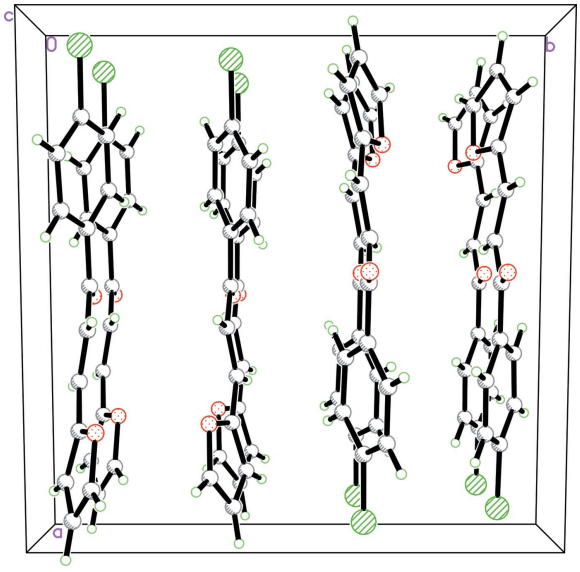


**Figure 2**
The crystal packing of (I), viewed down the $c$ axis.

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