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1-(2-Furyl)-3-phenyl-2-propen-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.079
Data-to-parameter ratio = 14.8

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

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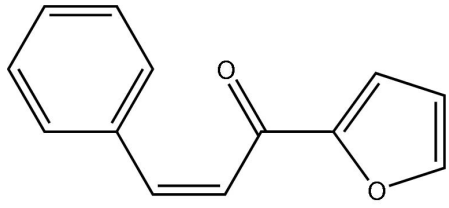
The molecule of the title compound, $C_{13}H_{10}O_2$ is nearly planar; the furyl and and phenyl rings are only slightly twisted with respect to each other, making a dihedral angle of 8.56 (6)°. The crystal structure is stabilized by weak intermolecular C—H···O contacts and C—H···π interactions.

Comment

The title compound, (I), is a derivative of chalcone (1,3-diphenyl-2-propen-1-one). Depending on the substitution pattern on the two aromatic rings, chalcones display an impressive array of pharmacological activities, including antiprotozoal (Nielsen *et al.*, 1998; Li *et al.*, 1995; Liu *et al.*, 2001), anti-inflammatory (Hsieh *et al.*, 1998), nitric oxide inhibition (Rojas *et al.*, 2002) and anticancer. Numerous clinically successful anticancer drugs are themselves either natural products or have been developed from naturally occurring lead compounds (Ducki *et al.*, 1998); activities have been cited in the literature.



(I)

The title compound is nearly planar, the furyl and phenyl rings making a dihedral angle of only 8.56 (6)°. Within the two rings, the maximum deviations are 0.007 (2) and 0.003 (2) Å for C3 and C13, respectively. The bond lengths in the furyl ring

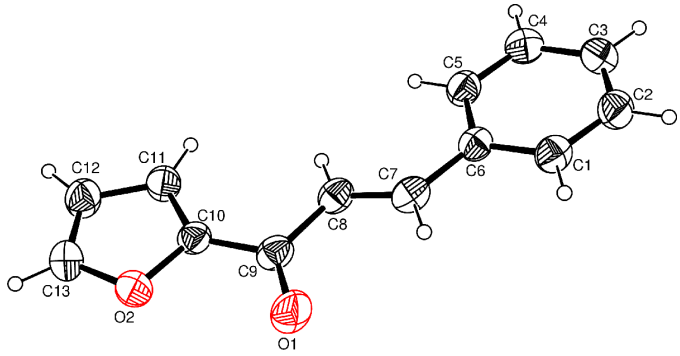


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

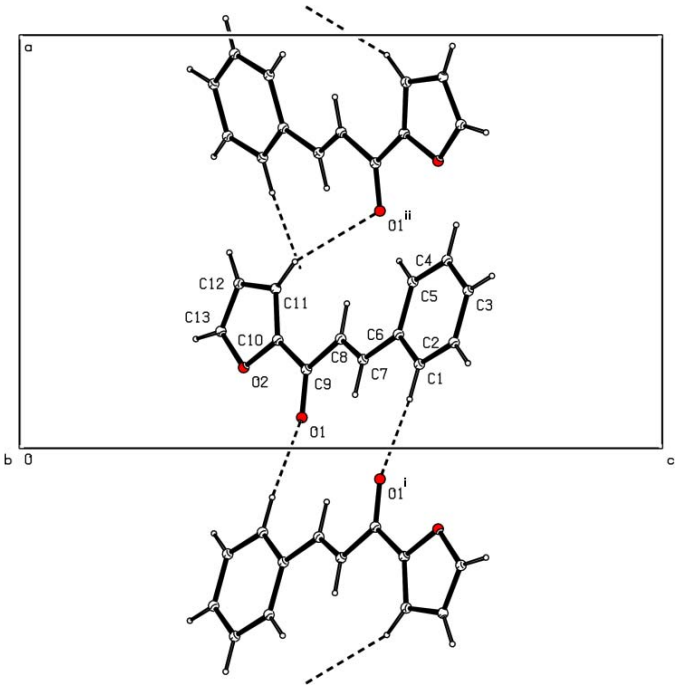


Figure 2
View of the chain along the *b* axis formed by C—H···O interactions (dashed lines) [symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$].

are in the normal range and are consistent with those in a related structure (Hernandez *et al.*, 1996).

The structure of (I) contains intermolecular C—H···O contacts, which link the molecule into discrete pairs across inversion centres (Table 1, Fig. 2). Further C—H···O interactions result in the formation of a chain along the *b* axis. There are also C—H···π interactions (Table 1).

Experimental

2-Acetylfuran (0.01 mol) and benzaldehyde (0.01 mol) were dissolved in ethanol (25 ml), put in an ice bath and stirred. Sodium hydroxide (0.5 g; 0.0125 mol) dissolved in water (2.5 ml) was then added dropwise to the cooled solution, not allowing the temperature to exceed 303 K during this mixing process. Then, keeping the temperature between 288 and 303 K, the solution was stirred for 3 h. The resulting precipitate was filtered off and washed with water and ethanol. After drying, (I) was crystallized from ethanol.

Crystal data

$C_{13}H_{10}O_2$
M_r = 198.21
Orthorhombic, *Pbca*
a = 10.4874 (10) Å
b = 12.1216 (14) Å
c = 16.3091 (16) Å
V = 2073.3 (4) Å^3
Z = 8
D_x = 1.270 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12064 reflections
θ = 1.7–29.1°
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colourless
0.80 × 0.47 × 0.09 mm

Data collection

Stoe IPDS 2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
T_{min} = 0.942, T_{max} = 0.989
13565 measured reflections
2034 independent reflections
1020 reflections with $I > 2\sigma(I)$
R_{int} = 0.100
θ_{max} = 26.0°
$h = -12 \rightarrow 12$
$k = -14 \rightarrow 14$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.079
S = 0.84
2034 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0154 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.93	2.48	3.347 (2)	156
C11—H11···O1^{ii}	0.93	2.52	3.345 (2)	149
C13—H13···$Cg2^{iii}$	0.93	2.58	3.410 (2)	149

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$; (iii) $x, -\frac{1}{2}-y, z-\frac{3}{2}$. *Cg*2 is the centroid of C1–C6.

All H atoms were included in calculated positions and treated using a riding model [C—H(aromatic) = 0.93 Å; U_{iso}(H) = 1.2U_{eq}(C)].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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