

## 5-(2-Furyl)-3-hydroxy-1-phenylpenta-2,4-dien-1-one

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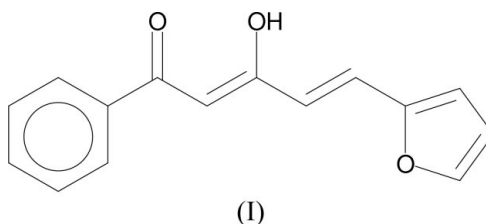
## Key indicators

Single-crystal X-ray study  
T = 105 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002 \text{ \AA}$   
R factor = 0.030  
wR factor = 0.062  
Data-to-parameter ratio = 14.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

In the crystalline state, the title molecule,  $\text{C}_{15}\text{H}_{12}\text{O}_3$ , exists in the enolized form and displays a strong intramolecular hydrogen bond. The molecular structure supports the hypothesis that the conjugation in the molecule is a determining factor for the position of the enol H atom. The packing of the molecules shows interactions between phenyl H atoms and enol groups, thus forming weak  $\text{C}-\text{H}\cdots\text{O}$  bonds. Possible  $\text{C}-\text{H}\cdots\pi$  interactions are also indicated.

## Comment

As a continuation of our study of curcuminoid compounds (Tønnesen *et al.*, 1982; Mostad, 1994; Arrieta & Mostad, 2004), we report here the crystal and molecular structure of the title compound, (I) (Fig. 1, Table 1).



In (I), atoms C1–C9, as well as the three O atoms, are almost coplanar, deviating from the mean plane by less than 0.07 Å. This mean plane and the phenyl ring make a dihedral angle of 20.5 (1)°. The enol H atom is bonded to atom O2, in accordance with the formation of the longest possible conjugated chain within the molecule. The O2–H distance is 1.00 (2) Å and the O1–H distance is 1.54 (2) Å. The enol character of O2 is also corroborated by the bond-length pattern within the enol group.

The packing of the molecules of (I) in the crystal structure is shown in Fig. 2, where the most prominent interaction between molecules,  $\text{C11}-\text{H11}\cdots\text{O1}^i$ , is shown (Table 2; symmetry code as in Table 2). This appears to be a good example of a  $\text{C}-\text{H}\cdots\text{O}$  interaction.

Finally, the arrangement of molecules III and IV relative to the central molecule indicate  $\text{C}-\text{H}\cdots\pi$  interactions between atoms H7 and H9 and the furanyl rings III and IV, respectively (Fig. 3; symmetry codes as in Fig. 3). The distances from H7 and H9 to the centres of the respective furanyl rings are 3.04 Å and 3.08 Å. The dihedral angles between the furanyl ring planes are 63.2 (2)° and 74.6 (2)°, respectively. The geometry of the contacts between H7 and H9 and the nearest atoms in the respective furanyl rings is given in Table 2.

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## Experimental

The title compound was synthesized from benzoylacetone and furan-2-aldehyde (Arrieta *et al.*, 1992). Deep-yellow prismatic-shaped crystals crystallized from absolute ethanol (m.p. 352–353 K).

## Crystal data

$C_{15}H_{12}O_3$   
 $M_r = 240.25$   
 Orthorhombic,  $Pbca$   
 $a = 11.0108(6) \text{ \AA}$   
 $b = 7.8652(4) \text{ \AA}$   
 $c = 27.999(1) \text{ \AA}$   
 $V = 2424.8(2) \text{ \AA}^3$   
 $Z = 8$   
 $D_x = 1.316 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation  
 Cell parameters from 7171 reflections  
 $\theta = 2.0\text{--}28.4^\circ$   
 $\mu = 0.09 \text{ mm}^{-1}$   
 $T = 105(2) \text{ K}$   
 Prismatic, yellow  
 $0.4 \times 0.2 \times 0.2 \text{ mm}$

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1997)  
 $T_{\min} = 0.964$ ,  $T_{\max} = 0.982$   
 27 362 measured reflections

3020 independent reflections  
 1514 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.081$   
 $\theta_{\text{max}} = 28.3^\circ$   
 $h = -14 \rightarrow 14$   
 $k = -10 \rightarrow 10$   
 $l = -36 \rightarrow 37$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.062$   
 $S = 0.74$   
 3020 reflections  
 211 parameters

All H-atom parameters refined  
 $w = 1/[\sigma^2(F_o^2) + (0.0295P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.11 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.17 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1—C1	1.271 (1)	C3—C4	1.452 (2)
O2—C3	1.337 (1)	C4—C5	1.337 (2)
O3—C9	1.374 (1)	C5—C6	1.431 (2)
O3—C6	1.380 (1)	C6—C7	1.361 (2)
C1—C2	1.430 (2)	C7—C8	1.417 (2)
C1—C10	1.475 (2)	C8—C9	1.334 (2)
C2—C3	1.370 (2)		
C9—O3—C6	106.1 (1)	C4—C5—C6	126.0 (1)
O1—C1—C2	119.6 (1)	C7—C6—O3	109.0 (1)
O1—C1—C10	118.7 (1)	C7—C6—C5	132.6 (1)
C2—C1—C10	121.8 (1)	O3—C6—C5	118.4 (1)
C3—C2—C1	121.4 (1)	C6—C7—C8	107.4 (1)
O2—C3—C2	121.5 (1)	C9—C8—C7	106.4 (1)
O2—C3—C4	116.1 (1)	C8—C9—O3	111.1 (1)
C2—C3—C4	122.5 (1)	C11—C10—C1	121.8 (1)
C5—C4—C3	123.4 (1)	C15—C10—C1	119.2 (1)
O1—C1—C10—C11	160.6 (1)	O1—C1—C10—C15	−17.0 (2)
C2—C1—C10—C11	−19.6 (2)	C2—C1—C10—C15	162.8 (1)

Table 2

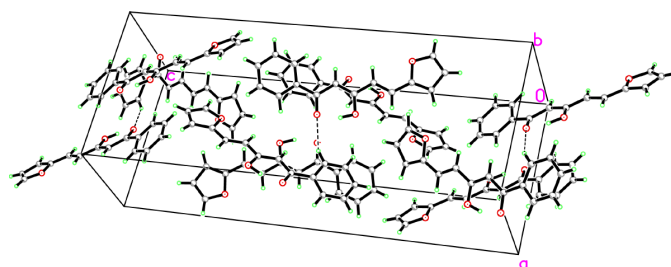
Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O2—H20 $\cdots$ O1	1.00 (2)	1.54 (2)	2.500 (1)	159 (1)
C11—H11 $\cdots$ O1 <sup>i</sup>	0.99 (1)	2.39 (1)	3.294 (2)	152 (1)
C9—H9 $\cdots$ C7 <sup>ii</sup>	0.97 (1)	2.86 (1)	3.748 (2)	154 (9)
C7—H7 $\cdots$ O3 <sup>iii</sup>	0.96 (1)	3.06 (1)	3.760 (2)	131 (1)

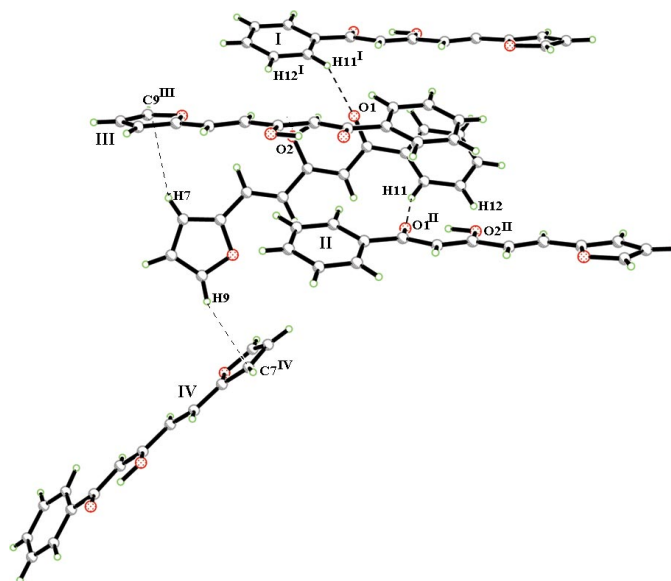
Symmetry codes: (i)  $\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$ ; (ii)  $2 - x, y - \frac{1}{2}, \frac{3}{2} - z$ ; (iii)  $\frac{3}{2} - x, \frac{1}{2} + y, z$ .



**Figure 1**  
 A view of the molecule of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.



**Figure 2**  
 The packing of the molecules of (I) in the unit cell. Hydrogen bonds are shown as dashed lines.



**Figure 3**  
 The interaction between the molecules of (I) in the crystal structure. [Symmetry codes: (I)  $x - \frac{1}{2}, \frac{1}{2} - y, 1 - z$ ; (II)  $\frac{1}{2} + x, \frac{1}{2} - y, 1 - z$ ; (III)  $\frac{3}{2} - x, \frac{1}{2} + y, z$ ; (IV)  $2 - x, y - \frac{1}{2}, \frac{3}{2} - z$ .]

All H atoms were located in difference Fourier maps and refined in an isotropic approximation. The C—H distances are in the range 0.93 (1)–1.02 (1)  $\text{\AA}$ .

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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