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1-(2-Furyl)-3-hydroxy-3-(4-phenylphenyl)-prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.003 Å
R factor = 0.058
wR factor = 0.158
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.

In the title compound, $C_{19}H_{14}O_3$, two independent molecules exist in the enol form with normal values for bond lengths and angles. The crystal packing is stabilized by van der Waals forces.

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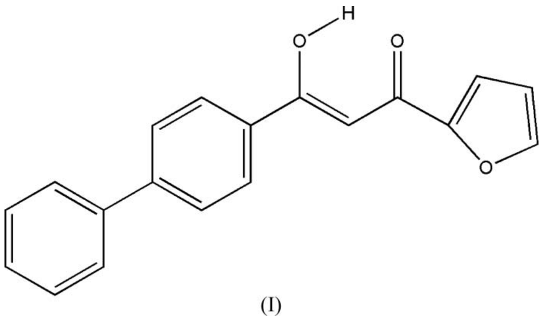
Comment

1,3-Diketones have been studied extensively in coordination chemistry (Ma *et al.*, 1999; Yoshida *et al.*, 2005). These compounds are often used as intermediates in syntheses (Hasegawa *et al.*, 1997; Morris *et al.*, 1996). 1,3-Diketones generally exist in enol and keto forms; the enol form is stabilized by the stronger intramolecular hydrogen bond (Vila *et al.*, 1991). We present here the crystal structure of the title compound, (I), a new 1,3-diketone.



(I)

Two independent molecules of (I) (Fig. 1) exist in the enol form, stabilized by intramolecular hydrogen bonds (Table 1). The conformations of the two molecules are slightly different: the central benzene ring (C7–C12) makes dihedral angles of 27.66 (9) and 8.43 (11)° with rings C1–C6 and O3/C16–C19, respectively, in one molecule; the corresponding angles in the other molecule are 26.89 (10) and 18.36 (11)°, respectively. The crystal packing is stabilized by van der Waals forces.

Experimental

1-(Biphenyl-4-yl)ethanone (5.88 g, 0.03 mol), methyl furan-2-carboxylate (4.41 g, 0.035 mol), $NaNH_2$ (1.56 g, 0.04 mol) and dry diethyl ether (40 ml) were placed into round-bottomed flask. The mixture was stirred for 6 h at room temperature under nitrogen, and then acidified with dilute hydrochloric acid; stirring was continued until all solids had dissolved. The ether layer was separated and washed with saturated $NaHCO_3$ solution, dried over anhydrous Na_2SO_4, and the solvent was removed by evaporation. The residual solid was recrystallized from ethanol to give the title compound (I) (yield 5.36 g, 61.6%; m.p. 381 K). Crystals suitable for X-ray diffraction were grown by slow evaporation of a CH_2Cl_2–EtOH (2:1) solution at room temperature.

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Crystal data

$C_{19}H_{14}O_3$
$M_r = 290.30$
Triclinic, $P\overline{1}$
$a = 9.9489$ (10) Å
$b = 10.4042$ (11) Å
$c = 16.1706$ (17) Å
$\alpha = 90.113$ (2)°
$\beta = 100.547$ (3)°
$\gamma = 116.292$ (3)°
$V = 1468.7$ (3) Å^3
$Z = 4$
$D_x = 1.313$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 297$ (2) K
Needle, yellow
0.30 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.983$, $T_{\max} = 0.994$
9454 measured reflections
5972 independent reflections
4868 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 26.5$°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.158$
$S = 1.07$
5972 reflections
403 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2 + 0.2029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.30$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4*A*···O5	0.87 (1)	1.68 (2)	2.5026 (19)	157 (3)
O1—H1*A*···O2	0.86 (1)	1.70 (2)	2.518 (2)	157 (3)

The C-bound H atoms were included in idealized positions (C—H = 0.93 Å) and allowed to ride during subsequent refinement, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$. Atoms H1*A* and H4*A* of the hydroxy groups were located in a difference Fourier map. In the free refinement, with $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm O})$, atoms H1*A* and H4*A* were positioned between two O atoms with O1—H1*A* = 0.99 (3), O2—H1*A* = 1.58 (3), O4—H4*A* = 1.09 (2) and O5—H4*A* = 1.46 (2) Å; these bond lengths are in agreement with those observed in related structures involving tautomeric equilibrium (Bertolasi *et al.*, 1991; Gilli *et al.*, 2004; Wang *et al.*, 2006). However, in view of the room-temperature experiment, in the final refinement the hydroxy H atoms were refined with the restraint O—H = 0.85 (1) Å.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

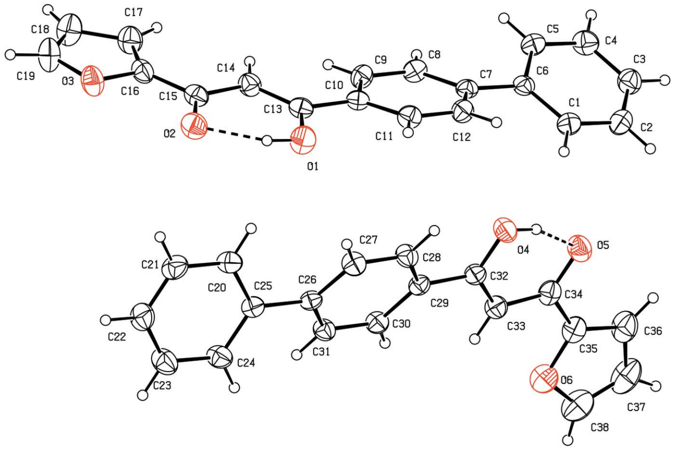

Figure 1
The asymmetric unit of (I), with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. The dashed lines indicate the intramolecular hydrogen bonds.

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