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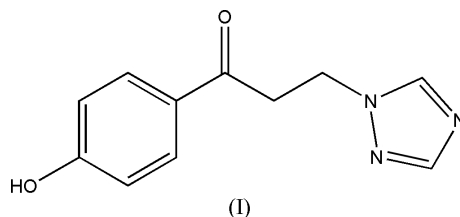
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.030
 wR factor = 0.076
Data-to-parameter ratio = 8.5For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.1-(4-Hydroxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)-propan-1-one

In the title compound, $\text{C}_{11}\text{H}_{11}\text{N}_3\text{O}_2$, the dihedral angles made by the planes of the triazole and benzene rings with the plane through the OC_3 atoms of the ketone group are $72.87(4)$ and $7.10(3)^\circ$, respectively. There are some intermolecular interactions in the crystal structure, which contribute to the stability.

Comment

Triazole rings appear frequently in the structures of various natural products and biologically active compounds, notably thiamine (vitamin B), penicillins and antibiotics, such as micrococcin (James & Watson, 1966). Triazole derivatives have also attracted considerable attention in industry and agriculture because of their significant biological activities (Zhang *et al.*, 2002). In this paper, we report the structure of the title compound (I).



In the title compound (Fig. 1), the bond lengths and angles are generally normal in the benzene and triazole rings (Ji *et al.*, 2002). The $\text{C}=\text{O}$ bond length is close to the typical $\text{C}=\text{O}$ double-bond length (Table 1). Atom C3 lies in the plane of the triazole ring, and atoms O1, C1, C2 and C6 are coplanar (plane p_1). The dihedral angles formed by the triazole and $\text{C6}-\text{C11}$ rings with p_1 are $72.87(4)$ and $7.10(3)^\circ$, respectively. The $\text{C2}-\text{C3}-\text{N1}-\text{N2}$, $\text{O1}-\text{C1}-\text{C2}-\text{C3}$, $\text{C7}-\text{C6}-\text{C1}-\text{O1}$ and $\text{C5}-\text{N1}-\text{C3}-\text{C2}$ torsion angles are $68.2(2)$, $4.1(3)$, $172.0(2)$ and $112.7(2)^\circ$, respectively. The most interesting structural features of the title compound are $\text{O}-\text{H}\cdots\text{N}$ intermolecular

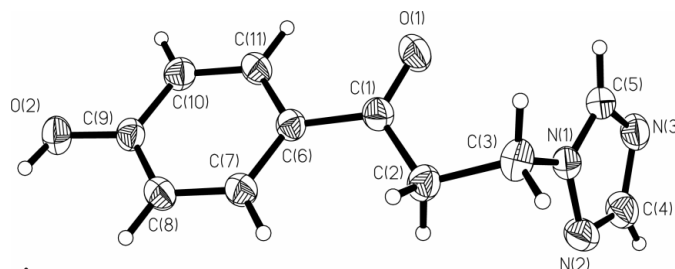


Figure 1
The structure of the title compound, showing 35% probability displacement ellipsoids and the atom-numbering scheme.

Received 11 January 2005

Accepted 12 January 2005

Online 22 January 2005

hydrogen bonds and weak (C—H...Y hydrogen bonds; Y = O and N) intermolecular interactions (see Table 2). These interactions stabilize the crystal structure.

Experimental

The title compound was prepared according to the method reported by Ogata *et al.* (1987). Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from methanol at room temperature.

Crystal data

C ₁₁ H ₁₁ N ₃ O ₂	$D_x = 1.356 \text{ Mg m}^{-3}$
$M_r = 217.23$	Mo $K\alpha$ radiation
Monoclinic, Cc	Cell parameters from 1098 reflections
$a = 22.759 (4) \text{ \AA}$	$\theta = 3.6\text{--}26.7^\circ$
$b = 5.5729 (9) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 8.3902 (14) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 90.929 (2)^\circ$	Block, colourless
$V = 1064.0 (3) \text{ \AA}^3$	$0.28 \times 0.22 \times 0.20 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	1271 independent reflections
φ and ω scans	1006 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.018$
$T_{\text{min}} = 0.958$, $T_{\text{max}} = 0.981$	$\theta_{\text{max}} = 27.9^\circ$
3413 measured reflections	$h = -29 \rightarrow 21$
	$k = -7 \rightarrow 7$
	$l = -9 \rightarrow 11$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.0744P]$
$R[F^2 > 2\sigma(F^2)] = 0.030$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.076$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.12 \text{ e \AA}^{-3}$
1271 reflections	$\Delta\rho_{\text{min}} = -0.13 \text{ e \AA}^{-3}$
149 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

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

N1—C3	1.459 (3)	C1—C6	1.476 (3)
O1—C1	1.218 (2)	C1—C2	1.513 (3)
O2—C9	1.347 (2)		
O1—C1—C2—C3	4.1 (3)	N2—N1—C3—C2	−68.2 (2)
C5—N1—C3—C2	112.7 (2)	O1—C1—C6—C7	−172.0 (2)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O2—H2...N3 ⁱ	0.857 (10)	1.834 (11)	2.685 (2)	172 (3)
C3—H3A...O1 ⁱⁱ	0.97	2.55	3.162 (3)	120
C3—H3B...N2 ⁱⁱⁱ	0.97	2.59	3.534 (3)	163
C4—H4...O2 ^{iv}	0.93	2.43	3.327 (3)	162
C5—H5...N2 ^v	0.93	2.51	3.389 (5)	157

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

H atoms on O atoms were located in a difference Fourier map and refined freely. All other H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 \AA , and included in the final cycles of refinement using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. In the absence of significant anomalous scattering, Friedel pairs were merged.

Data collection: SMART (Bruker, 1998); 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, 1999); software used to prepare material for publication: SHELXTL.

This project was supported by the National Natural Science Foundation of China (grant No. 40376023).

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