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1-(4-Methoxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)-propan-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.112
Data-to-parameter ratio = 10.9

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

In the title compound, $C_{12}H_{13}N_3O_2$, molecules are linked into layers parallel to $(\bar{1}01)$ by intermolecular C—H···O hydrogen bonds. The packing is further stabilized by C—H···π interactions.

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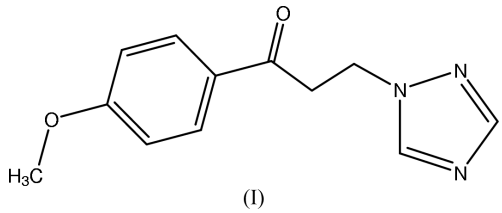
Comment

Many triazole compounds have good fungicidal and plant growth regulating activities (Xu *et al.*, 2002). In addition, according to empirical data (Xu *et al.*, 2004), the presence of an accessible triazole ring is conducive to improvement of the biological activity. To explore this idea, the title compound, (I), was synthesized and an X-ray crystallographic analysis was undertaken to establish the structure.



(I)

The bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and comparable with those in a related compound (Xu *et al.*, 2004). The bond distances in the triazole ring show a character intermediate between single and double bonds (Table 1). The non-H atoms of the molecule are nearly coplanar (r.m.s. deviation = 0.129 Å), with a dihedral angle between the two aromatic rings of 11.15 (7)°. In the crystal structure, molecules are linked by C11—H11···O2^{i} and C12—H12···O1^{ii} intermolecular hydrogen bonds to form a layer parallel to $(\bar{1}01)$ (Fig. 2; for symmetry codes see Table 2) The packing is further stabilized by C—H···π interactions involving the benzene ring.

Experimental

The title compound was prepared according to the literature method of Shi *et al.* (1996). Colourless single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethyl acetate–petroleum ether (1:1 *v*/*v*) solution over a period of two weeks.

Crystal data

$C_{12}H_{13}N_3O_2$
M_r = 231.25
Monoclinic, $P2_1/c$
a = 8.2642 (13) Å
b = 11.4273 (18) Å
c = 12.0990 (19) Å
β = 94.709 (2)°
V = 1138.7 (3) Å^3
Z = 4
D_x = 1.349 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3530 reflections
θ = 2.5–25.9°
μ = 0.10 mm^{-1}
T = 293 (2) K
Block, colourless
0.42 × 0.33 × 0.21 mm

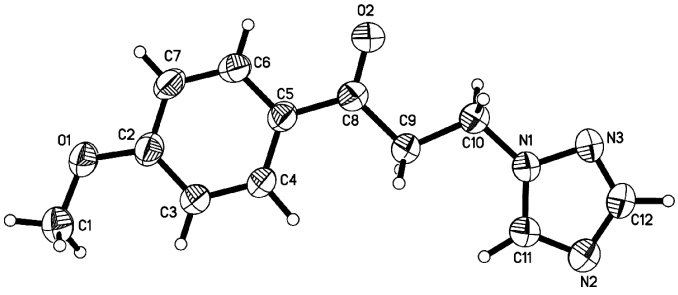


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	2238 independent reflections
ω scans	1976 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.014$
$T_{min} = 0.961$, $T_{max} = 0.980$	$\theta_{max} = 26.0^\circ$
6241 measured reflections	$h = -9 \rightarrow 10$
	$k = -14 \rightarrow 8$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.1229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.112$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.26$ e Å^{-3}
2238 reflections	
206 parameters	
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

O1—C2	1.3581 (14)	N1—C10	1.4605 (14)
O1—C1	1.4268 (17)	N2—C11	1.3240 (17)
O2—C8	1.2229 (15)	N2—C12	1.3412 (18)
N1—C11	1.3238 (16)	N3—C12	1.3110 (17)
N1—N3	1.3593 (13)		
C2—O1—C1	118.24 (10)	O2—C8—C9	120.05 (10)
O1—C2—C3	124.66 (11)	C5—C8—C9	118.79 (10)
O1—C2—C7	115.50 (10)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···O2^{i}	0.96 (2)	2.42 (2)	3.372 (2)	167 (1)
C12—H12···O1^{ii}	0.98 (1)	2.43 (1)	3.277 (2)	145 (1)
C1—H1C···$Cg1^{iii}$	0.97 (2)	2.78 (2)	3.607 (2)	143 (1)
C10—H10B···$Cg1^{iv}$	0.97 (2)	2.71 (2)	3.594 (2)	151 (1)

Symmetry codes: (i) $2-x, \frac{1}{2}+y, \frac{1}{2}-z$; (ii) $1+x, y, 1+z$; (iii) $1-x, 1-y, -z$; (iv) $x, \frac{1}{2}-y, \frac{1}{2}+z$. $Cg1$ is the centroid of the benzene ring.

All H atoms were located in difference Fourier maps and refined isotropically. C—H distances lie in the range 0.915 (15)–1.007 (16) Å.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); 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).

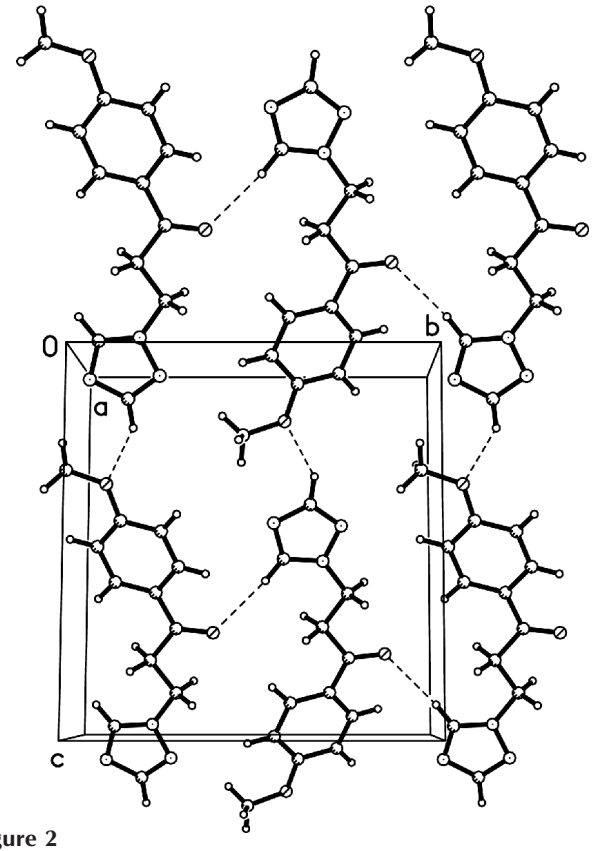


Figure 2
A view down the *a* axis of the layered structure of (I). Hydrogen bonds are indicated by dashed lines.

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