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

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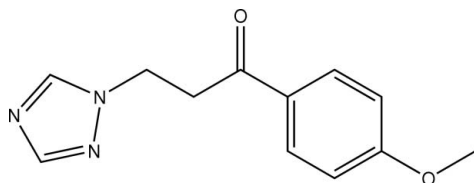Correspondence e-mail: qustchemistry@126.com

In the title compound, $C_{12}H_{13}N_3O_2$, the methoxyphenyl-propanone unit is approximately planar. The dihedral angle between the benzene ring and the triazole ring is 80.60 (1)°. A C—H···π interaction stabilizes the crystal structure.

Related literature

For related literature, see: Allen *et al.* (1987); Czollner *et al.* (1990); Feng *et al.* (1991); Gasztonyi & Josepovits (1984); Goswami *et al.* (1984); Xu *et al.* (2002).

Experimental

Crystal data

$C_{12}H_{13}N_3O_2$
$M_r = 231.25$
Monoclinic, $P2_1/c$
$a = 12.382$ (3) Å
$b = 9.852$ (3) Å
$c = 9.481$ (2) Å
$\beta = 92.542$ (4)°

$V = 1155.4$ (5) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 293$ (2) K
$0.36 \times 0.20 \times 0.15$ mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.967$, $T_{max} = 0.986$

6301 measured reflections
2284 independent reflections
1676 reflections with $I > 2\sigma(I)$
$R_{int} = 0.028$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.138$
$S = 1.03$
2284 reflections

154 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···$Cg1^i$	0.96	2.95	3.826 (3)	152

Symmetry code: (i) $x - 1, -y - \frac{1}{2}, z - \frac{1}{2}$. $Cg1$ is the centroid of the triazole ring.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2231).

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supplementary materials

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Comment

Over the years a great variety of triazole derivatives, especially 1,2,4-triazole compounds, have been synthesized due to their broad spectrum of biological properties, such as antiviral, antitumor, antifungal and plant-growth regulatory activities (Gasztonyi & Josepovits, 1984; Xu *et al.*, 2002; Czollner *et al.*, 1990; Goswami *et al.*, 1984; Feng *et al.*, 1991). Some of them have been commercially developed into highly efficient, hypotoxic, low-toxicity and inward-absorbing fungicides and plant-growth regulatory agents. In a search for new compounds with higher bioactivity, the title compound was synthesized as an intermediate and its structure is presented here.

In the molecule of the title compound, all the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The benzene ring (C1—C6) and triazole ring (N1—N3/C10/C11) make a dihedral angle of 80.60 (1)°. The crystal packing (Fig. 2) is stabilized by C—H···π interactions (Table 1) and van der Waals forces.

Experimental

A mixture of 1-(4-methoxyphenyl)ethanone (0.1 mol), dissolved in ethanol (30 ml), paraformaldehyde (0.11 mol), dimethyl-amine hydrochloride (0.11 mol) and hydrochloric acid (1 ml) as a catalyst were refluxed with stirring for *ca* 5 h. The white solid as the intermediate was obtained. To the intermediate (0.04 mol) dissolved in water triazole (0.03 mol, dissolve in water) was slowly dropped and the solution was kept for 5 h at room temperature. The reaction solution was extracted with chloroform and the product was obtained after chloroform was evaporated. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).
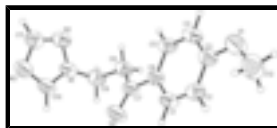
Figures

Fig. 1. The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom numbering scheme.
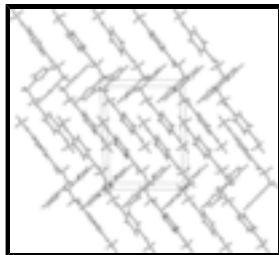
Fig. 2. A packing diagram of the title compound, viewed down the *b* axis.

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

Crystal data

$C_{12}H_{13}N_3O_2$	$F_{000} = 488$
$M_r = 231.25$	$D_x = 1.329$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 1736 reflections
$a = 12.382$ (3) Å	$\theta = 2.6–23.5º$
$b = 9.852$ (3) Å	$\mu = 0.09$ mm^{-1}
$c = 9.481$ (2) Å	$T = 293$ (2) K
$\beta = 92.542$ (4)º	Block, colourless
$V = 1155.4$ (5) Å^3	$0.36 \times 0.20 \times 0.15$ mm
$Z = 4$	

Data collection

Siemens SMART 1000 CCD area-detector diffractometer	2284 independent reflections
Radiation source: fine-focus sealed tube	1676 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.028$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 26.1º$
$T = 293(2)$ K	$\theta_{min} = 1.7º$
ω scans	$h = -15 \rightarrow 12$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$k = -10 \rightarrow 12$
$T_{min} = 0.967$, $T_{max} = 0.986$	$l = -11 \rightarrow 11$
6301 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H-atom parameters constrained
$wR(F^2) = 0.138$	$w = 1/[\sigma^2(F_o^2) + (0.0765P)^2 + 0.0537P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$

2284 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.20$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of F$^2 > 2$sigma(F^2) is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O2	0.82431 (11)	0.39787 (12)	0.08465 (14)	0.0690 (4)
N1	1.04168 (12)	0.22834 (13)	0.08435 (14)	0.0514 (4)
C7	0.79559 (14)	0.28218 (16)	0.11083 (17)	0.0500 (4)
C6	0.70459 (14)	0.25647 (15)	0.20236 (17)	0.0469 (4)
N3	1.16341 (13)	0.32367 (15)	0.22615 (18)	0.0647 (5)
O1	0.44700 (12)	0.18628 (13)	0.45845 (15)	0.0701 (4)
N2	1.08202 (14)	0.12623 (15)	0.16777 (16)	0.0628 (5)
C1	0.63630 (15)	0.36228 (16)	0.2358 (2)	0.0561 (5)
H1A	0.6490	0.4482	0.1995	0.067*
C3	0.53102 (15)	0.21624 (17)	0.37627 (18)	0.0526 (4)
C5	0.68374 (16)	0.12889 (16)	0.26002 (18)	0.0532 (5)
H5A	0.7280	0.0559	0.2395	0.064*
C4	0.59902 (16)	0.10994 (16)	0.34628 (19)	0.0569 (5)
H4A	0.5872	0.0247	0.3849	0.068*
C2	0.55067 (16)	0.34386 (17)	0.3208 (2)	0.0569 (5)
H2B	0.5060	0.4165	0.3412	0.068*
C11	1.15354 (16)	0.18920 (19)	0.2493 (2)	0.0602 (5)
H11A	1.1950	0.1442	0.3189	0.072*
C10	1.09170 (17)	0.34256 (17)	0.1218 (2)	0.0623 (5)
H10A	1.0777	0.4262	0.0793	0.075*
C9	0.95636 (16)	0.20091 (18)	−0.02167 (19)	0.0588 (5)
H9A	0.9785	0.1273	−0.0819	0.071*
H9B	0.9447	0.2808	−0.0802	0.071*
C8	0.85212 (15)	0.16316 (18)	0.04473 (19)	0.0569 (5)
H8A	0.8672	0.0950	0.1168	0.068*
H8B	0.8037	0.1230	−0.0268	0.068*
C12	0.38215 (19)	0.2934 (2)	0.5066 (3)	0.0833 (7)
H12A	0.3267	0.2571	0.5634	0.125*

supplementary materials

H12B	0.3494	0.3405	0.4270	0.125*
H12C	0.4263	0.3553	0.5620	0.125*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O2	0.0774 (9)	0.0369 (7)	0.0937 (10)	−0.0068 (6)	0.0168 (8)	0.0069 (6)
N1	0.0630 (9)	0.0368 (7)	0.0553 (8)	−0.0022 (6)	0.0126 (7)	0.0020 (6)
C7	0.0592 (11)	0.0368 (9)	0.0533 (10)	−0.0043 (7)	−0.0069 (8)	0.0030 (7)
C6	0.0562 (10)	0.0337 (8)	0.0499 (9)	−0.0043 (7)	−0.0062 (8)	0.0012 (7)
N3	0.0682 (10)	0.0478 (9)	0.0784 (11)	−0.0070 (8)	0.0050 (9)	0.0021 (8)
O1	0.0746 (9)	0.0586 (8)	0.0787 (9)	−0.0068 (7)	0.0206 (7)	0.0039 (7)
N2	0.0799 (11)	0.0399 (8)	0.0690 (10)	0.0007 (8)	0.0058 (9)	0.0031 (7)
C1	0.0659 (12)	0.0334 (9)	0.0689 (12)	−0.0019 (8)	0.0012 (10)	0.0075 (7)
C3	0.0598 (11)	0.0459 (10)	0.0517 (10)	−0.0068 (8)	−0.0004 (9)	0.0003 (7)
C5	0.0668 (12)	0.0341 (9)	0.0585 (10)	0.0010 (8)	0.0000 (9)	0.0013 (7)
C4	0.0754 (13)	0.0338 (9)	0.0618 (11)	−0.0060 (8)	0.0051 (10)	0.0075 (7)
C2	0.0623 (11)	0.0385 (9)	0.0700 (11)	0.0038 (8)	0.0040 (10)	0.0015 (8)
C11	0.0648 (12)	0.0516 (11)	0.0649 (12)	0.0027 (9)	0.0103 (10)	0.0027 (9)
C10	0.0739 (13)	0.0373 (9)	0.0761 (13)	−0.0054 (9)	0.0075 (11)	0.0060 (9)
C9	0.0763 (13)	0.0473 (10)	0.0533 (10)	−0.0030 (9)	0.0090 (9)	−0.0025 (8)
C8	0.0684 (12)	0.0440 (10)	0.0583 (10)	−0.0070 (8)	0.0029 (9)	−0.0035 (8)
C12	0.0778 (15)	0.0805 (16)	0.0932 (16)	−0.0016 (12)	0.0241 (13)	−0.0031 (13)

Geometric parameters (Å, °)

O2—C7	1.2226 (19)	C3—C2	1.389 (2)
N1—C10	1.325 (2)	C5—C4	1.371 (3)
N1—N2	1.3609 (19)	C5—H5A	0.9300
N1—C9	1.451 (2)	C4—H4A	0.9300
C7—C6	1.474 (3)	C2—H2B	0.9300
C7—C8	1.515 (2)	C11—H11A	0.9300
C6—C1	1.388 (2)	C10—H10A	0.9300
C6—C5	1.399 (2)	C9—C8	1.508 (3)
N3—C10	1.313 (2)	C9—H9A	0.9700
N3—C11	1.349 (2)	C9—H9B	0.9700
O1—C3	1.360 (2)	C8—H8A	0.9700
O1—C12	1.414 (3)	C8—H8B	0.9700
N2—C11	1.306 (2)	C12—H12A	0.9600
C1—C2	1.372 (3)	C12—H12B	0.9600
C1—H1A	0.9300	C12—H12C	0.9600
C3—C4	1.381 (2)		
C10—N1—N2	108.46 (16)	C3—C2—H2B	120.2
C10—N1—C9	131.39 (15)	N2—C11—N3	115.72 (17)
N2—N1—C9	120.14 (14)	N2—C11—H11A	122.1
O2—C7—C6	121.10 (16)	N3—C11—H11A	122.1
O2—C7—C8	119.57 (17)	N3—C10—N1	111.97 (16)
C6—C7—C8	119.31 (14)	N3—C10—H10A	124.0

C1—C6—C5	117.44 (17)	N1—C10—H10A	124.0
C1—C6—C7	119.64 (14)	N1—C9—C8	111.55 (14)
C5—C6—C7	122.92 (16)	N1—C9—H9A	109.3
C10—N3—C11	101.46 (15)	C8—C9—H9A	109.3
C3—O1—C12	118.88 (16)	N1—C9—H9B	109.3
C11—N2—N1	102.39 (15)	C8—C9—H9B	109.3
C2—C1—C6	121.95 (16)	H9A—C9—H9B	108.0
C2—C1—H1A	119.0	C9—C8—C7	113.67 (15)
C6—C1—H1A	119.0	C9—C8—H8A	108.8
O1—C3—C4	116.25 (16)	C7—C8—H8A	108.8
O1—C3—C2	124.41 (17)	C9—C8—H8B	108.8
C4—C3—C2	119.34 (17)	C7—C8—H8B	108.8
C4—C5—C6	120.97 (17)	H8A—C8—H8B	107.7
C4—C5—H5A	119.5	O1—C12—H12A	109.5
C6—C5—H5A	119.5	O1—C12—H12B	109.5
C5—C4—C3	120.60 (16)	H12A—C12—H12B	109.5
C5—C4—H4A	119.7	O1—C12—H12C	109.5
C3—C4—H4A	119.7	H12A—C12—H12C	109.5
C1—C2—C3	119.69 (17)	H12B—C12—H12C	109.5
C1—C2—H2B	120.2		
O2—C7—C6—C1	13.5 (2)	C2—C3—C4—C5	−1.5 (3)
C8—C7—C6—C1	−164.65 (15)	C6—C1—C2—C3	0.3 (3)
O2—C7—C6—C5	−165.64 (16)	O1—C3—C2—C1	−178.23 (16)
C8—C7—C6—C5	16.2 (2)	C4—C3—C2—C1	0.8 (3)
C10—N1—N2—C11	0.14 (19)	N1—N2—C11—N3	−0.1 (2)
C9—N1—N2—C11	−178.74 (14)	C10—N3—C11—N2	0.0 (2)
C5—C6—C1—C2	−0.6 (3)	C11—N3—C10—N1	0.1 (2)
C7—C6—C1—C2	−179.81 (16)	N2—N1—C10—N3	−0.2 (2)
C12—O1—C3—C4	172.62 (17)	C9—N1—C10—N3	178.53 (16)
C12—O1—C3—C2	−8.3 (3)	C10—N1—C9—C8	−111.3 (2)
C1—C6—C5—C4	−0.1 (3)	N2—N1—C9—C8	67.3 (2)
C7—C6—C5—C4	179.08 (15)	N1—C9—C8—C7	73.46 (19)
C6—C5—C4—C3	1.1 (3)	O2—C7—C8—C9	13.4 (2)
O1—C3—C4—C5	177.61 (16)	C6—C7—C8—C9	−168.47 (14)

Hydrogen-bond geometry (Å, °)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C12—H12A⋯Cg1[i]	0.96	2.95	3.826 (3)	152

Symmetry codes: (i) *x*−1, −*y*−1/2, *z*−1/2.

Fig. 1

Fig. 2