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1-(4,5-Dihydro-3-*p*-tolyl-1*H*-pyrazol-1-yl)-2-(1,2,4-triazol-1-yl)ethanone

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.121
Data-to-parameter ratio = 15.2

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

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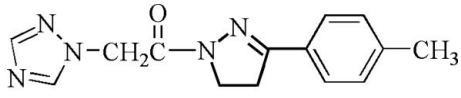
In the title compound, $C_{14}H_{15}N_5O$, the benzene and triazole rings are almost perpendicular and the dihedral angle between the pyrazole and triazole rings is 79.63 (3)°. There are some weak intermolecular C—H···O hydrogen-bond interactions in the crystal structure, which provide stabilization.

Comment

Triazole derivatives are known to have good and extensive insecticidal, fungicidal, herbicidal and acaricidal activity (Xu *et al.*, 2004; Blass *et al.*, 2003). Until now, studies on triazole derivatives have mainly concentrated on compounds with triazole as the only active group, whereas reports on triazole compounds containing both triazole and other active groups in the same molecule are rare. It is also know that pyrazoles and their derivatives have biological properties, such as medicinal and pesticidal activity (Angermann & Franke, 2001; Kordik *et al.*, 2001). In a search for better herbicidal and fungicidal activity, the title compound, (I), which contains both triazole and pyrazole groups, was synthesized and the structure investigated.



(I)

A molecular view of (I) is shown in Fig. 1. The bond lengths and angles within the benzene and triazole rings are in agreement with values observed in related compounds (Ji *et al.*, 2003; Liu *et al.*, 2002). The C3═N2 bond length of 1.283 (2) Å is close to the typical C═N double-bond length (1.34 Å; Allen *et al.*, 1987). Atom C12 lies in the plane of the triazole ring, the mean deviation from the least-squares plane

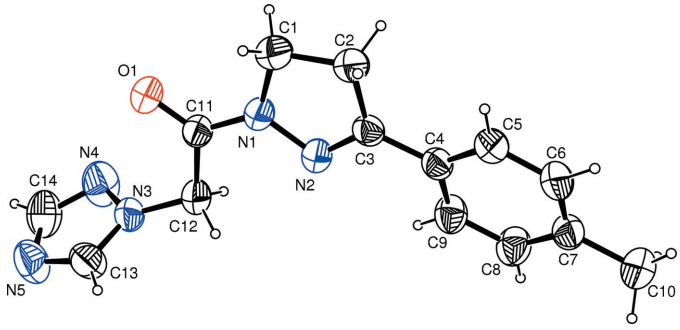


Figure 1
View of the title compound (I) with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii.

being 0.009 (4) Å. The pyrazole ring is roughly planar, with the largest deviation being 0.027 (1) Å for atom C1. The dihedral angles formed by the benzene and the triazole rings with the pyrazole ring are 13.50 (12) and 79.63 (6)°, respectively. Some weak C—H···O intermolecular hydrogen-bond interactions stabilize the crystal packing (Fig. 2 and Table 1).

Experimental

A mixture of 2-(1*H*-1,2,4-triazol-1-yl)acetohydrazide (0.02 mol), 1-phenyl-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one (0.02 mol) and *p*-toluenesulfonic acid (0.002 mol) was stirred in refluxing 2-propanol (20 ml) for 16 h at 355.4 K to afford the title compound. Single crystals suitable for X-ray measurements were obtained by recrystallization from an acetone–ethanol (1:2 *v*/*v*) solution at room temperature.

Crystal data

$C_{14}H_{15}N_5O$	D_x = 1.315 Mg m^{-3}
M_r = 269.31	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 1785 reflections
a = 5.2398 (10) Å	θ = 2.3–25.9°
b = 17.978 (3) Å	μ = 0.09 mm^{-1}
c = 14.476 (3) Å	T = 294 (2) K
β = 94.064 (3)°	Block, white
V = 1360.2 (4) Å^3	0.22 × 0.16 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2772 independent reflections
	1619 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.032
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 26.4°
	$h = -6 \rightarrow 3$
T_{min} = 0.970, T_{max} = 0.988	$k = -22 \rightarrow 22$
7599 measured reflections	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.1972P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	
$wR(F^2)$ = 0.121	
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
2772 reflections	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
182 parameters	$\Delta\rho_{min}$ = −0.14 e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···O1^{i}	0.93	2.55	3.474 (3)	171
C13—H13···O1^{ii}	0.93	2.52	3.304 (3)	142

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

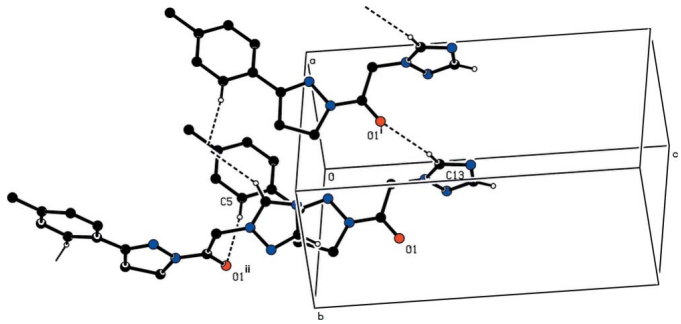


Figure 2
View of the C—H···O hydrogen bonds, shown as dashed lines. [Symmetry codes: (i) $x, \frac{3}{2}-y, z-\frac{1}{2}$; (ii) $1+x, y, z$.]

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) for the aryl and methylene H atoms and 1.5U_{eq}(C) for the methyl H atoms.

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: *ORTEPIII* (Burnett & Johnson, 1996) and *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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