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1-(4-Methylphenyl)-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) = 0.003 Å
R factor = 0.037
wR factor = 0.108
Data-to-parameter ratio = 8.4

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

In the title compound, $C_{12}H_{13}N_3O$, the benzene and triazole rings make a dihedral angle of 59.6 (2)°. The crystal packing is stabilized by weak C—H···π interactions and van der Waals forces.

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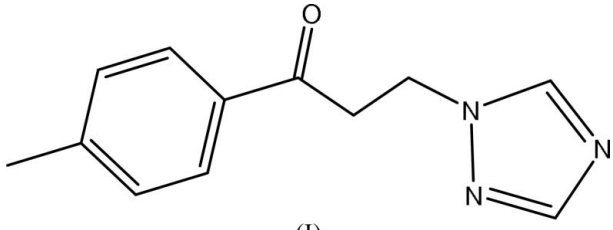
Comment

In our ongoing studies of triazole compounds, the title compound, (I), was obtained in the reaction of triazole and 3-(dimethylamino)-1-(4-methylphenyl)-propan-1-one hydrochloride. We report its crystal structure here.



(I)

The bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987) and are comparable with those in related compounds (Wan, Li, Li & Zhang, 2005; Wan, Li, Li, Li *et al.*, 2005). The molecular skeleton of (I) is non-planar, with a dihedral angle of 59.6 (2)° between the benzene and triazole rings.

There is a weak intramolecular C9—H9*A*···N2 hydrogen bond (Table 2). The crystal packing is stabilized by weak intermolecular C—H···π interactions (Table 2) and van der Waals forces.

Experimental

Triazole (3.5 g, 0.58 mol) was added to a solution of 3-(dimethylamino)-1-(4-methylphenyl)propan-1-one hydrochloride (11.4 g, 0.05 mol) in water (30 ml). The mixture was heated under reflux for 4 h, yielding a copious precipitate. Colourless single crystals of (I) suitable for X-ray diffraction study were obtained by slow evaporation of an ethyl acetate–petroleum ether (1:1, (*v*/*v*) solution over a period of two weeks.

Crystal data

$C_{12}H_{13}N_3O$
M_r = 215.25
Orthorhombic, $Pca2_1$
a = 10.943 (4) Å
b = 13.777 (5) Å
c = 7.514 (3) Å
V = 1132.8 (7) Å^3
Z = 4
D_x = 1.262 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 2634 reflections
θ = 2.4–25.2°
μ = 0.08 mm^{-1}
T = 293 (2) K
Block, colourless
0.45 × 0.26 × 0.12 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.963, T_{max} = 0.990
5789 measured reflections
1220 independent reflections
1067 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 26.2°
$h = -12 \rightarrow 13$
$k = -13 \rightarrow 16$
$l = -9 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.108
S = 1.14
1220 reflections
146 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2 + 0.0695P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 1997)
Extinction coefficient: 0.024 (4)

Table 1
Selected bond lengths (Å).

O1—C8	1.215 (3)	N2—C11	1.311 (4)
N1—C12	1.323 (4)	N3—C12	1.321 (4)
N1—N2	1.350 (3)	N3—C11	1.325 (5)
N1—C10	1.460 (3)		

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

*Cg*1 is the centroid of the triazole ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*A*···N2	0.97	2.63	2.988 (3)	102
C12—H12*A*···*Cg*1^{i}	0.93	2.67	3.571 (3)	135

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

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and with U_{iso}(H) = 1.2–1.5U_{eq}(C). Friedel pairs were merged before the final refinement.

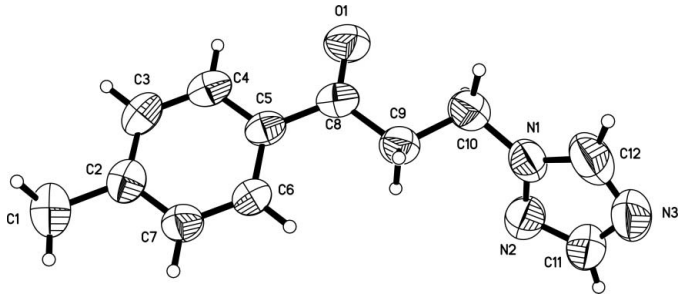


Figure 1
A view of (I), showing the atom-numbering scheme and 50% probability displacement ellipsoids.

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).

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