Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2,3-Dimethylphenoxy)-1-(pyridin-2-yl)-2-(1*H*-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) = 0.004 Å
R factor = 0.044
wR factor = 0.126
Data-to-parameter ratio = 12.9

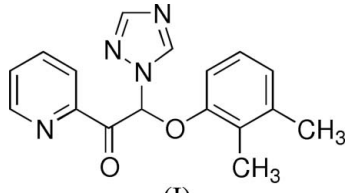
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{17}H_{16}N_4O_2$, a potent fungicidal agent, has been synthesized and its crystal structure determined. The dihedral angles between the planes of the pyridinyl and triazole rings, and between the substituted phenyl and triazole rings are 82.7 (2)° and 77.0 (3)°, respectively.

Received 9 September 2005
Accepted 22 September 2005
Online 28 September 2005

Comment

It is well known that compounds containing the 1*H*-1,2,4-triazole ring system are highly active as fungicides (Buchenauer, 1979), especially against the *Basidiomycete* and *Ascomycete* groups of fungi. These compounds are known to inhibit the biosynthesis of ergosterol in fungi (Hiroshi *et al.*, 1995; Fang *et al.*, 2003*a*,*b*). They are widely applied in the fields of medication and plant protection. In addition, compounds containing the pyridinyl ring are becoming more and more important in the development of medicines and fungicides, due to their excellent biological activities (Xiong *et al.*, 2001; Zhao *et al.*, 2004; Kurahashi *et al.*, 1997; Wagner *et al.*, 2000).



(I)

As a continuation of our interest in searching for novel 1*H*-1,2,4-triazole compounds with potent fungicidal activities, we have sought to synthesize 1*H*-1,2,4-triazole compounds involving pyridinyl units. We report here the structure of 2-(2,3-dimethylphenoxy)-1-(pyridin-2-yl)-2-(1*H*-1,2,4-triazol-1-yl)ethanone, (I).

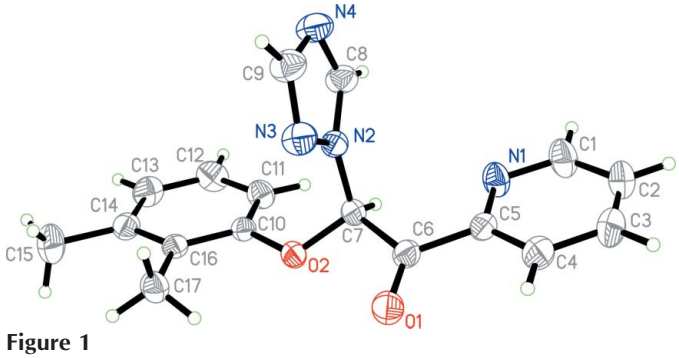


Figure 1
View of the title compound, with displacement ellipsoids drawn at the 30% probability level.

Fig.1 shows the molecular structure of (I); it contains three planar ring systems, *viz*. the pyridinyl ring (*p*1), the triazole ring (*p*2) and the substituted phenyl ring (*p*3). The dihedral angles between *p*1 and *p*2, and between *p*3 and *p*2 are 82.7 (2)° and 77.0 (3)°, respectively. The bond lengths and bond angles are unexceptional.

Experimental

2-Bromo-1-(pyridin-2-yl)-2-(1*H*-1,2,4-triazol-1-yl)ethanone hydrobromide (5 mmol) was dissolved in acetone (15 ml). A mixture of 2,3-dimethylphenol (6 mmol), Et_3N (10 mmol) and acetone (20 ml) was then added dropwise, while cooling on an ice-bath. The reaction mixture was stirred at room temperature for 2.5 h (monitored by TLC). The solution was filtered, and the filtrate was evaporated under reduced pressure. The residue was dissolved in 25 ml chloroform and washed with water (3 × 20 ml) and then adjusted to pH = 7 with 2 N aqueous NaOH. The organic layer was separated and washed with water (3 × 20 ml). The combined organic layer was dried over anhydrous Na_2SO_4. After removal of the solvent, the residue was separated by column chromatography on silica gel (200–300 mesh, with petroleum ether/ethyl acetate (4:1 *v*/*v*) as eluant, and recrystallized from petroleum ether/ethyl acetate (1:1 *v*/*v*) to give a yellow crystal (yield 62%).

Crystal data

$C_{17}H_{16}N_4O_2$	$Z = 2$
$M_r = 308.34$	$D_x = 1.312$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 7.700$ (2) Å	Cell parameters from 1220 reflections
$b = 9.989$ (3) Å	$\theta = 2.8$–$24.3°$
$c = 11.230$ (3) Å	$\mu = 0.09$ mm^{-1}
$\alpha = 102.490$ (4)°	$T = 294$ (2) K
$\beta = 108.484$ (4)°	Hexagonal fragment, yellow
$\gamma = 97.688$ (4)°	0.24 × 0.18 × 0.10 mm
$V = 780.5$ (3) Å^3	

Data collection

Bruker SMART 1000 CCD area detector diffractometer	2728 independent reflections
	1738 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.019$
Absorption correction: multi-scan *SADABS* (Sheldrick, 1996)	$\theta_{max} = 25.0°$
	$h = -9 \rightarrow 8$
$T_{min} = 0.978$, $T_{max} = 0.991$	$k = -9 \rightarrow 11$
3976 measured reflections	$l = -12 \rightarrow 13$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0632P)^2 + 0.0431P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.044$	
$wR(F^2) = 0.126$	$(\Delta/\sigma)_{max} = 0.004$
$S = 1.03$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
2728 reflections	$\Delta\rho_{min} = -0.20$ e Å^{-3}
211 parameters	Extinction correction: *SHELXL97*
H-atom parameters constrained	Extinction coefficient: 0.045 (6)

All H atoms were placed in calculated positions and were refined isotropically, with $U_{iso}(H) = 1.2U_{eq}(C)$, using a riding model with C—H = 0.93–0.98 Å.

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*.

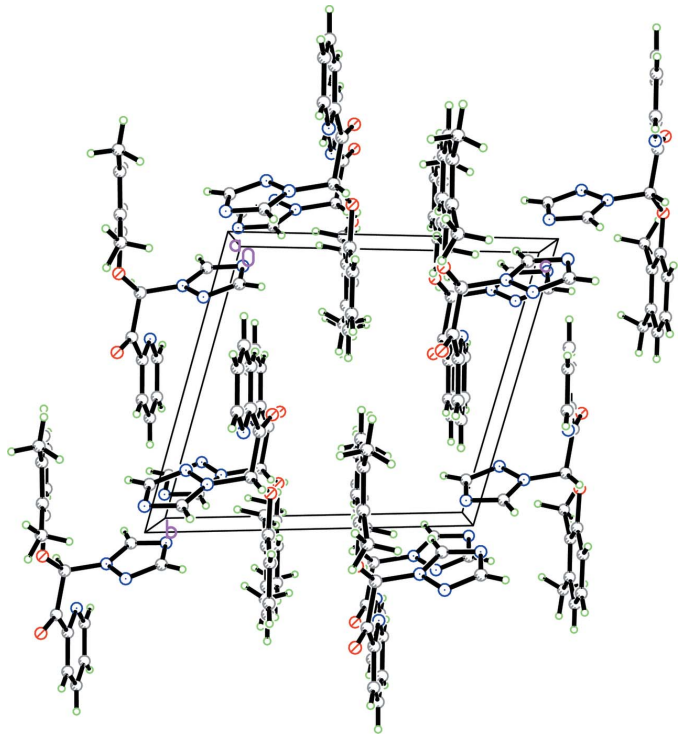


Figure 2
Packing diagram of the title compound.

This work was supported by the National Natural Science Foundation of China (NNSFC) (No.29872022, 20172030) and the Key Project of the Chinese Ministry of Education (No.105046).

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