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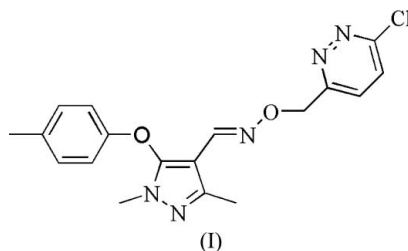
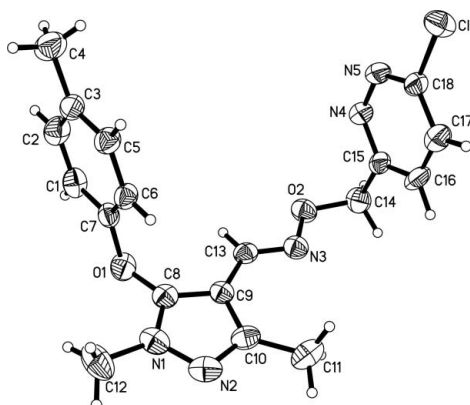
Key indicators

Single-crystal X-ray study
T = 294 K
Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
R factor = 0.055
wR factor = 0.187
Data-to-parameter ratio = 13.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**(*E*)-1,3-Dimethyl-5-*p*-tolylloxy-1*H*-pyrazole-4-carbaldehyde *O*-(6-chloropyridazin-3-yl)oxime**In the title molecule, C₁₈H₁₈ClN₅O₂, the central pyrazole ring is perpendicular to the benzene ring and approximately perpendicular to the pyridazine ring [dihedral angles 89.9 (2) and 82.8 (2)°, respectively].

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Comment

Many pyridazine derivatives have been found to exhibit biological activities such as insecticidal, fungicidal, herbicidal, plant-growth regulatory activity, *etc.* (Heinisch & Kopelent, 1992). For example, pyridate, credazine and maleic hydrazide (Kolar & Tisler, 1999) have been commercialized as herbicides. In order to discover new biologically active pyridazine compounds, the title compound, (I), was synthesized and its structure is reported here.In the molecule of (I) (Fig. 1), the central pyrazole ring is perpendicular to the benzene ring [dihedral angle = 89.9 (2)°] and approximately perpendicular to the pyridazine ring [dihedral angle = 82.8 (2)°]. The C13/N3/O2/C14 linkage is planar within 0.042 (2) Å and it is twisted away from the pyrazole ring by 14.8 (1)°. Bond lengths and angles are comparable to those found for (*E*)-5-(3,5-dimethylphenoxy)-1,3-dimethyl-1*H*-pyrazole-4-carbaldehyde *O*-(2-chloropyrimidin-4-yl)oxime (Zou *et al.*, 2006). The crystal packing is stabilized by C—H...O interactions (Table 1). A short**Figure 1**
The molecular structure of (I), showing 30% probability displacement ellipsoids.

C11...N2($-\frac{1}{2} + x, y, \frac{1}{2} - z$) contact of 3.187 (4) Å is also observed.

Experimental

3-Bromomethyl-6-chloropyridazine (2.2 mmol), anhydrous potassium carbonate (0.552 g, 4 mmol), and 1,3-dimethyl-5-*p*-tolylxy-1*H*-pyrazole-4-carbaldehyde oxime (2 mmol) were mixed in acetonitrile (40 ml) and refluxed for 5 h. The solvent was then evaporated *in vacuo*. The residue was recrystallized from ethanol and single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from acetone at room temperature.

Crystal data

C ₁₈ H ₁₈ ClN ₅ O ₂	Z = 8
<i>M_r</i> = 371.82	<i>D_x</i> = 1.312 Mg m ⁻³
Orthorhombic, <i>Pbca</i>	Mo <i>K</i> α radiation
<i>a</i> = 14.866 (3) Å	<i>μ</i> = 0.23 mm ⁻¹
<i>b</i> = 10.499 (2) Å	<i>T</i> = 294 (2) K
<i>c</i> = 24.121 (5) Å	Block, colourless
<i>V</i> = 3764.7 (12) Å ³	0.30 × 0.26 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	17909 measured reflections
<i>φ</i> and <i>ω</i> scans	3320 independent reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 1996)	1606 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T_{min}</i> = 0.936, <i>T_{max}</i> = 0.956	<i>R_{int}</i> = 0.070
	<i>θ_{max}</i> = 25.0°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0543P)^2 + 6.5016P]$
$R[F^2 > 2\sigma(F^2)] = 0.055$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.187$	(Δ/σ) _{max} = 0.002
<i>S</i> = 1.02	$\Delta\rho_{\text{max}} = 0.40 \text{ e } \text{Å}^{-3}$
3320 reflections	$\Delta\rho_{\text{min}} = -0.24 \text{ e } \text{Å}^{-3}$
238 parameters	
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C16—H16...O2 ⁱ	0.93	2.50	3.409 (6)	166

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

All H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å, and included in the final cycles of refinement using a riding model, with *U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq}(methyl C)

Data collection: *SMART* (Bruker, 1999); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; 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*.

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