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4-(4-*tert*-Butylphenoxy)-2-chloropyrimidine

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
Disorder in main residue
R factor = 0.055
wR factor = 0.134
Data-to-parameter ratio = 15.3

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

In the title compound, $C_{14}H_{15}ClN_2O$, the benzene and pyrimidine rings are nearly perpendicular, the dihedral angle between them being 84.7 (2)°.

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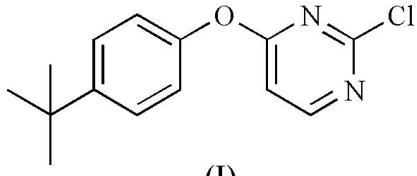
Comment

Pyrimidine derivatives are very important molecules in biology and have many applications in the areas of pesticide and pharmaceutical agents (Condon *et al.*, 1993). For example, imazosulfuron, ethirmol and mepanipyrim have been commercialized as agrochemicals (Maeno *et al.*, 1990). Pyrimidine derivatives have also been developed as antiviral agents, such as AZT, which is the most widely used anti-AIDS drug (Gilchrist, 1997). In order to discover further biologically active pyrimidine compounds, the title compound, (I), was synthesized and its crystal structure determined (Fig. 1).



(I)

The benzene and pyrimidine rings of (I) are nearly perpendicular, the dihedral angle between them being 84.7 (2)°. The C3—C4—O1—C5, N1—C4—O1—C5, C10—C5—O1—C4 and C6—C5—O1—C4 torsion angles are 6.8 (4), −174.0 (3), −93.2 (3) and 91.2 (3)°, respectively (Table 1).

Experimental

2,4-Dichloropyrimidine (0.30 g, 2 mmol) and anhydrous potassium carbonate (0.35 g, 2.5 mmol) were mixed in acetone (20 ml). A solution of 4-*tert*-butylphenol (0.32 g, 2.1 mmol) in acetone (5 ml) was then added dropwise with stirring. The mixture was stirred at room temperature overnight. The solvent was then evaporated *in vacuo* and the residue was washed with water. The resulting light-yellow precipitate was filtered off and recrystallized from ethanol and well shaped crystals of (I) were obtained.

Crystal data

$C_{14}H_{15}ClN_2O$
M_r = 262.73
Monoclinic, *C*2/*c*
a = 20.692 (11) Å
b = 12.456 (6) Å
c = 11.792 (6) Å
β = 114.510 (8)°
V = 2765 (2) Å^3
Z = 8
D_x = 1.262 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 602 reflections
θ = 2.2–21.2°
μ = 0.27 mm^{-1}
T = 294 (2) K
Block, yellow
0.20 × 0.18 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.932, T_{max} = 0.958
6731 measured reflections
2788 independent reflections
1384 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 26.3°
$h = -25 \rightarrow 25$
$k = -9 \rightarrow 15$
$l = -12 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.134
S = 1.00
2788 reflections
182 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0558P)^2 + 0.1813P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C4	1.354 (3)	N2—C2	1.336 (3)
O1—C5	1.406 (3)	C2—C3	1.365 (3)
N2—C1	1.310 (3)		
C6—C5—O1	119.5 (3)	C5—C6—C7	119.4 (3)
C10—C5—O1	119.7 (3)		
C1—N1—C4—O1	−179.9 (2)	C4—O1—C5—C6	91.2 (3)
C1—N1—C4—C3	−0.7 (4)	C4—O1—C5—C10	−93.2 (3)
C5—O1—C4—N1	−174.0 (3)	O1—C5—C6—C7	175.2 (2)
C5—O1—C4—C3	6.8 (4)	O1—C5—C10—C9	−174.8 (2)
C2—C3—C4—O1	179.7 (3)		

The three methyl groups show positional disorder. At the final stage of the refinement, the occupancy factors of two possible sites, C12/C13/C14 and C12′/C13′/C14′, were fixed at 0.87 and 0.13, respectively. H atoms were placed in calculated positions and treated as riding atoms, with C—H = 0.93 Å (aromatic H) or 0.96 Å (methyl H), and U_{iso}(H) = 1.2U_{eq}(C) or U_{iso}(H) = 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); 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*.

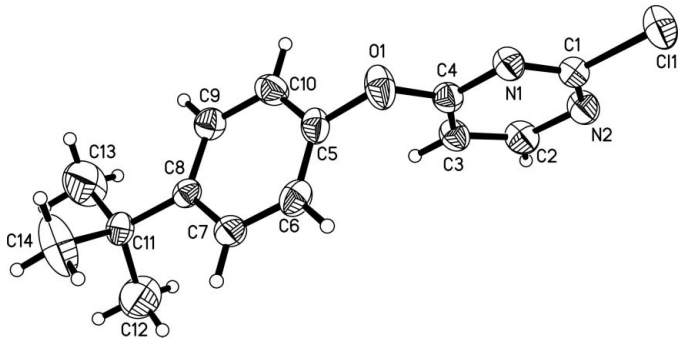


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Only the major component of the disorder is shown.

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