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2-*tert*-Butylamino-1-(4-chlorophenyl)-4,4-dimethyl-1*H*-imidazolin-5(4*H*)-one

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.123
Data-to-parameter ratio = 18.4

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

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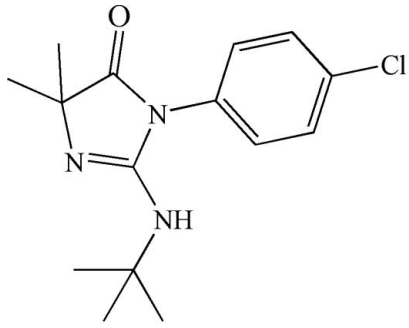
In the title compound, $C_{15}H_{20}ClN_3O$, the five-membered ring and the amino N atom are essentially coplanar.

Comment

Derivatives of imidazolinone have shown biological and pharmaceutical activities (Sulkowski *et al.*, 1997). Some have exhibited good antibacterial and antifungal activities (Trivedi *et al.*, 2002). In recent years, we have been engaged in the preparation of derivatives of heterocycles *via* the aza-Wittig reaction (Ding *et al.*, 2004). The title compound, (I), was synthesized and structurally characterized in this context.



(I)

Atom N3 and the five-membered ring are essentially coplanar (Fig. 1), the maximum deviation being 0.0006 Å for atom N3, and the mean deviation from this plane is 0.0142 Å. The dihedral angle between this plane and the benzene ring is 114.3 (2)°. The bond lengths involving atom C7 indicate a degree of electron delocalization (Yang *et al.*, 1999). Selected bond lengths and angles are listed in Table 1 and a packing diagram is shown in Fig. 2.

Experimental

To a solution of iminophosphane (3 mmol) in dichloromethane (10 ml) was added a solution of phenyl isocyanate in dichloromethane (10 ml). The resulting solution was stirred for 1.5 h at 258 K. The reaction mixture was then purified by column chromatography on silica gel using petroleum ether–diethyl ether (25:1 *v*/*v*) as eluent to afford the intermediate carbodiimide, which was reacted with *tert*-butyl imide to give (I) in 56% yield (m.p. 413 K). ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.18–7.50 (*m*, 4H, PhH), 3.59 (*s*, 1H, NH), 1.42 (*s*, 9H, CH_3), 1.59 (*s*, 6H, CH_3). MS (EI, 70 eV) *m*/*z* (%): 294/293 (12/32), 236 (100), 221 (34), 152 (46), 127 (28), 56 (32). Crystals suitable for single-crystal X-ray diffraction were grown from a mixture of petroleum ether and dichloromethane (3:1 *v*/*v*) at 273 K.

Crystal data

$C_{15}H_{20}ClN_3O$
M_r = 293.79
Monoclinic, $P2_1/n$
a = 6.0758 (8) Å
b = 18.8340 (2) Å
c = 13.8603 (18) Å
β = 98.530 (2)°
V = 1568.5 (3) Å^3
Z = 4
D_x = 1.244 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2568 reflections
θ = 2.6–22.7°
μ = 0.24 mm^{-1}
T = 292 (2) K
Block, colourless
0.40 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
10046 measured reflections
3425 independent reflections
2208 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.0°
$h = -7 \rightarrow 7$
$k = -22 \rightarrow 24$
$l = -17 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.123
S = 0.98
3425 reflections
186 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.366 (3)	C7—N1	1.420 (2)
C3—C4	1.378 (3)	C8—N2	1.472 (2)
C4—C6	1.378 (3)	C8—C9	1.514 (3)
C5—C6	1.373 (2)	C9—O1	1.211 (2)
C6—N1	1.426 (2)	C9—N1	1.382 (2)
C7—N2	1.272 (2)	C12—N3	1.487 (2)
C7—N3	1.354 (2)		
C5—C6—C4	119.37 (17)	O1—C9—N1	125.24 (18)
C5—C6—N1	120.14 (16)	N1—C9—C8	105.81 (15)
C4—C6—N1	120.46 (16)	C9—N1—C7	107.06 (15)
N2—C7—N3	127.10 (16)	C9—N1—C6	125.00 (14)
N2—C7—N1	114.80 (15)	C7—N1—C6	127.84 (14)
N3—C7—N1	118.09 (16)	C7—N2—C8	107.38 (14)
N2—C8—C9	104.76 (14)		
N2—C7—N1—C9	0.1 (2)	C5—C6—N1—C7	117.96 (19)
N3—C7—N1—C9	178.79 (16)	C4—C6—N1—C7	−63.8 (2)
N2—C7—N1—C6	176.62 (16)	N3—C7—N2—C8	178.64 (18)
N3—C7—N1—C6	−4.7 (3)	N1—C7—N2—C8	−2.9 (2)
C5—C6—N1—C9	−66.2 (2)	N2—C7—N3—C12	−14.1 (3)
C4—C6—N1—C9	112.1 (2)	N1—C7—N3—C12	167.40 (15)

H atoms were placed at calculated positions and refined as riding (C—H = 0.93–0.96 Å and N—H = 0.86 Å), with U_{iso}(H) = 1.2 (CH, NH) or 1.5 (CH_3) times U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Bruker, 1997); software used to prepare material for publication: *SHELXTL-NT*.

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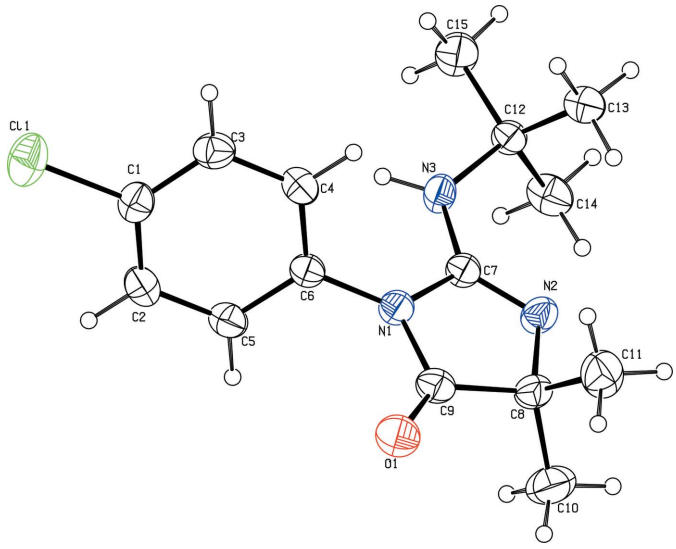

Figure 1
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

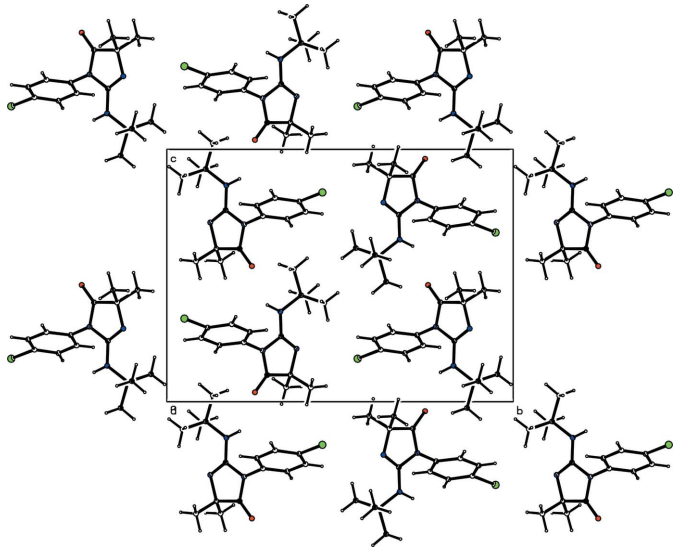

Figure 2
Packing diagram for (I), viewed down the *a* axis.

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