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# (*Z*)-4-Benzylidene-1-(4-chlorophenyl)-2-propylamino-1*H*-imidazol-5(4*H*)-one

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**Key indicators**

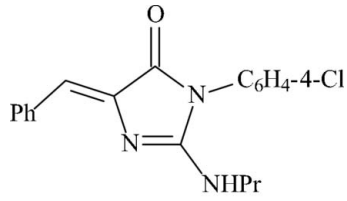
Single-crystal X-ray study
*T* = 292 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
*R* factor = 0.052
*wR* factor = 0.139
Data-to-parameter ratio = 16.5

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

Adjacent molecules of the title compound, $C_{19}H_{18}ClN_3O$, are linked by an N···O hydrogen bond [2.926 (2) Å] into a zigzag chain.

## Comment

Several PhCH═C($CO_2$Et)N═C═N*R* (*R* = Ph, 4-Cl$C_6H_4$) compounds that were synthesized from an aza-Wittig reaction of PhCH═C($CO_2$Et)N═P$Ph_3$ with *R*NCO have been reacted with primary amines to form 1-aryl-2-alkylamino-4-benzylideneimidazolin-5-ones (Ding *et al.*, 2001). Among these is the title compound (I) (Fig. 1), whose amino group is hydrogen-bonded with the carbonyl group of an adjacent molecule (Table 1), forming a zigzag chain running along the *c* axis. The compound features an imidazolinone unit with an exocyclic C═C double bond.




(I)

There are few related compounds whose structures have been determined. The examples appear to be limited to (4*Z*)-4-(4-methoxybenzylidene)-1,2-diphenyl-1,4-dihydro-5-imidazolin-5-one (Bhattacharjya *et al.*, 2004), 1-[2-(dimethylamino)ethyl]-2-methyl-4-benzylidene-2-imidazolin-5-one (Oshimi *et al.*, 2002) and (*Z*)-1-[2-(dimethylamino)ethyl]-2-methyl-4-benzylidene-2-imidazolin-5-one (Kawasaki *et al.*, 2004).

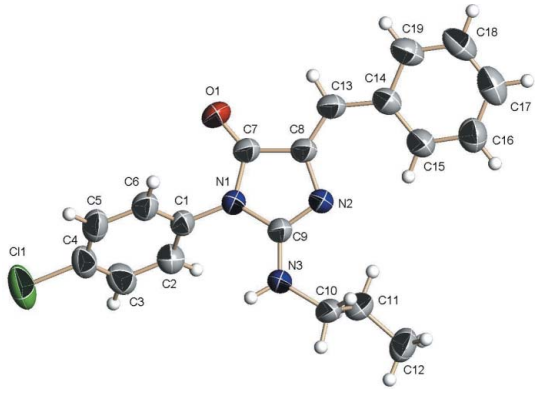



**Figure 1**
The molecular structure of (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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## Experimental

The compound was synthesized according to a reported procedure (Ding *et al.*, 2001) and crystals were grown from a dichloromethane/diethyl ether solution (1:1 *v*/*v*).

*Crystal data*

$C_{19}H_{18}ClN_3O$
$M_r$ = 339.81
Monoclinic, $P2_1/c$
$a$ = 10.9150 (7) Å
$b$ = 12.9335 (8) Å
$c$ = 12.8701 (8) Å
$\beta$ = 103.331 (1)°
$V$ = 1767.9 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.277 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.23 mm$^{-1}$
$T$ = 292 (2) K
Block, yellow
0.2 × 0.2 × 0.2 mm

*Data collection*

Bruker SMART APEX area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
16744 measured reflections
4038 independent reflections
2612 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.050
$\theta_{max}$ = 27.5°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.139
$S$ = 0.97
4038 reflections
245 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N3—H3$n$···O1$^{i}$ | 0.86 | 2.15 | 2.926 (2) | 150 |
| N3—H3$n'$···O1$^{i}$ | 0.86 | 2.36 | 2.926 (2) | 124 |

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

The propyl chain is disordered over two positions; the occupancy factors refined to 0.612 (6):0.388 (2). The pairs of 1,2-related and 1,3-related distances were restrained to be equal within 0.01 Å. H atoms were positioned geometrically and were included in the refinement in the riding-model approximation [aryl C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C); methylene C—H = 0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C); methyl C—H = 0.96 Å and $U_{iso}$(H) = 1.5$U_{eq}$(C)]. Because of disorder of the propyl group, the H atom bonded to atom N3 is disordered over two sites (H3$n$ and H3$n'$), which were refined in riding mode, with N—H = 0.86 Å and $U_{iso}$(H) = 1.2$U_{eq}$(N).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); 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, 1998); software used to prepare material for publication: *SHELXL97*.

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