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4-Benzylidene-1-phenyl-2-propylamino-1*H*-imidazol-5(4*H*)-one

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In the title compound, $C_{19}H_{19}N_3O$, the five-membered imidazolone ring is essentially planar. Intermolecular N—H···O hydrogen bonds form an infinite chain. The C—N and C—C bond lengths indicate electron delocalization.

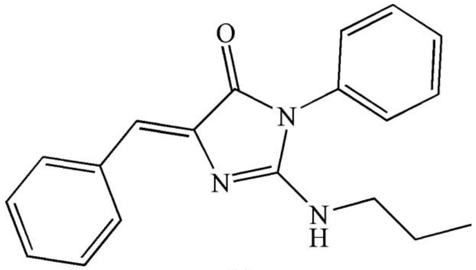
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.054
wR factor = 0.143
Data-to-parameter ratio = 17.8

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

Comment

Imidazolones are important heterocycles having fungicidal, anti-inflammatory and angiotensin II antagonist activities (Lacroix *et al.*, 2000). Some 2-alkylaminoimidazolones exhibit good antibacterial activity (Trivedi *et al.*, 2002). The title compound, (I), may be used as a new precursor for obtaining bioactive molecules.



(I)

The molecular structure of (I) is shown in Fig. 1. The five-membered imidazolone ring is planar. Benzene ring C1–C6 is only slightly twisted with respect to this imidazolone ring, making a dihedral angle of 4.46 (9)°. The C7—C8 bond length of 1.347 (2) Å is close to that of a typical C═C bond (1.35 Å), whereas the N1—C10 bond length of 1.3047 (19) Å, is slightly longer than that of a typical C═N bond (1.28 Å). The N3—C10, N2—C10, N2—C11 and N2—C9 bond lengths [1.3292 (19), 1.4004 (18), 1.426 (2) and 1.3860 (19) Å, respectively] indicate some degree of delocalization around the ring system (Yang *et al.*, 1999). The C6—C7—C8—N1 torsion angle of 0.6 (3)° indicates a *Z* configuration of the molecule about the C7═C8 bond.

Intermolecular N—H···O hydrogen bonds (Table 1) link the molecules into chains, as can be seen from the packing diagram (Fig. 2).

Experimental

To a solution of vinyliminophosphorane (3 mmol) in dry dichloromethane (10 ml) was added phenyl isocyanate (3 mmol) under nitrogen at room temperature. After 8 h, the solvent was removed under reduced pressure and a mixture of diethyl ether/petroleum ether (1:2 *v*/*v*, 20 ml) was added to precipitate triphenylphosphine oxide. After the mixture was filtered, the filtrate was condensed and

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dichloromethane (10 ml) was added to make a solution of carbodiimide, which was added to *n*-propylamine (3 mmol). After 2 h, the solvent was removed under reduced pressure and the residual was recrystallized from dichloromethane/ethanol to give (I) in 67% yield (m.p. 456 K). ^{1}H NMR (CDCl$_3$, 400 MHz): δ 8.16–7.10 (*m*, 10H, Ar—H), 6.70 (*s*, 1H, =CH), 4.58(*t*, 1H, *J* = 5.4 Hz, NH), 3.60–3.38 (*m*, 2H, NCH$_2$), 1.85–1.45 (*m*, 2H, CH$_2$), 0.94 (*t*, 3H, *J* = 7.2 Hz, CH$_3$); MS (EI 70 eV) *m*/*z*(%): 305(M^+, 95%), 276 (64%), 263 (96%), 119 (100%). Elemental analysis calculated for $C_{19}H_{19}N_3O$: C 74.73, H 6.27, N 13.76%; found: 74.62, H 6.37, N 13.61%.

Crystal data

$C_{19}H_{19}N_3O$
$M_r = 305.37$
Monoclinic, $P2_1/c$
$a = 11.6442$ (11) Å
$b = 11.3675$ (10) Å
$c = 12.8149$ (12) Å
$\beta = 99.058$ (2)°
$V = 1675.1$ (3) Å^3
$Z = 4$
$D_x = 1.211$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3773 reflections
$\theta = 2.4$–23.8°
$\mu = 0.08$ mm^{-1}
$T = 292$ (2) K
Block, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
14038 measured reflections
3784 independent reflections
2657 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$
$\theta_{\rm max} = 27.5$°
$h = -14 \rightarrow 15$
$k = -14 \rightarrow 13$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.143$
$S = 1.06$
3784 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2 + 0.168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.16$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.16$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1$^{\rm i}$	0.871 (8)	2.094 (13)	2.8452 (17)	144.0 (16)

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

H atoms attached to carbon were placed at calculated positions and treated as riding atoms (C—H = 0.93–0.97 Å), with $U_{\rm iso}$ values set equal to 1.2$U_{\rm eq}$ (CH) or 1.5$U_{\rm eq}$(CH$_3$) of the parent atom. The H atom attached to nitrogen was refined with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(N).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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 2001) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

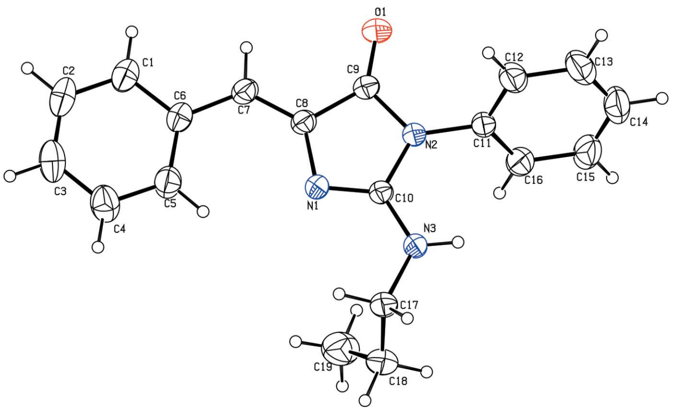

Figure 1
View of the molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

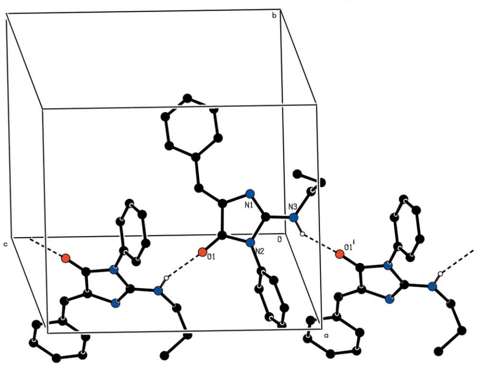

Figure 2
The hydrogen-bonding interactions in (I) forming a chain [symmetry code: (i) $x, \frac{1}{2}-y, z-\frac{1}{2}$]. H atoms not involved in hydrogen bonding have been omitted.

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References

Bruker (2001). *SMART* (Version 5.0), *SAINT* (Version 5.0) and *SHELXTL-NT* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Lacroix, G., Peignier, R., Pepin, R., Bascou, J. P., Perez, J. & Schmitz, C. (2000). US Patent No. 6002016; *Chem. Abstr.* (2000). **132**, 35698e.
Sheldrick G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Trivedi, S. D., Kubawat, H. T. & Parekh, H. H. (2002). *J. Indian Chem. Soc.* **79**, 282–283.
Yang, G. F., Liu, H. Y. & Yang, H. Z. (1999). *Sci. China Ser. B*, **42**, 656–662.