Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*E*)-3-Isopropyl-5,5-dimethyl-2-(phenylimino)-imidazolidin-4-one

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In the title compound, $C_{14}H_{19}N_3O$, intermolecular N—H···O hydrogen bonds form an infinite chain along the *a* axis. Electron delocalizition affects the C—N bonds.

Received 13 July 2005
Accepted 15 July 2005
Online 23 July 2005

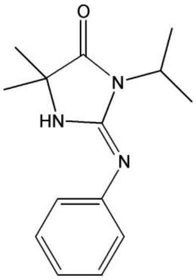
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.103
Data-to-parameter ratio = 9.2

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

Comment

Derivatives of imidazolones have shown biological and pharmaceutical activities (Sulkowski *et al.*, 1997). Some exhibit good antibacterial and antifungal activities (Trivedi *et al.*, 2002). The title compound, (I), may be used as a new precursor for obtaining bioactive molecules. The crystal structure of (I) is presented here.



(I)

Atoms N1, C7, N2, and N3 are coplanar (Fig. 1), the maximum deviation being 0.0001 Å for atom N3. The dihedral angle between this plane and the phenyl ring is 45 **(s.u.)**°. The C7—N1, C7—N2 and C7—N3 bond lengths are 1.276 (3), 1.356 (2) and 1.412 (3) Å, respectively, indicating a degree of electron delocalizition (Yang *et al.*, 1999). The N3—C7—N1—C6 torsion angle of −177.7 (2)° indicates an *E* configuration of the moleule about the C7═N1 bond.

The intermolecular interaction N2—H2*A*···O1 (*H*···*A* = 2.25 Å, N···O = 2.951 (2) Å and N2—H2*A*···O1 = 139°) forms a hydrogen-bond chain (Fig. 2).

Experimental

A solution of phenyl isocyanate in dry dichloromethane (10 ml) was added to a solution of iminophosphane (3 mmol) in dichloromethane (10 ml). The resulting solution was stirred for 1.5 h at 258 K. The resoluted mixture was then purified by column chromatography on silica gel, with petroleum ether/diethyl ether (25:1 *v*/*v*) as eluent to afford the intermediate carbodiimide, which was reacted with isopropylimide to give (I) in 56% yield. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 6.96–7.35 (*m*, 5H, Ph-H), 4.55–4.58 (*m*, 2H, N—H, C12-H), 1.49–1.53 (*d*, 6H, C13-H, C14-H), 1.36 (*s*, 6H, CH_3); m.p. 442 K. MS (EI 70 eV) m/*z*(%): 159/158 (26/22), 118/117 (24/23), 77 (11), 42/41 (100/47). Crystals suitable for single-crystal X-ray diffraction were grown from petroleum ether at 273 K.

doi:10.1107/S1600536805022749

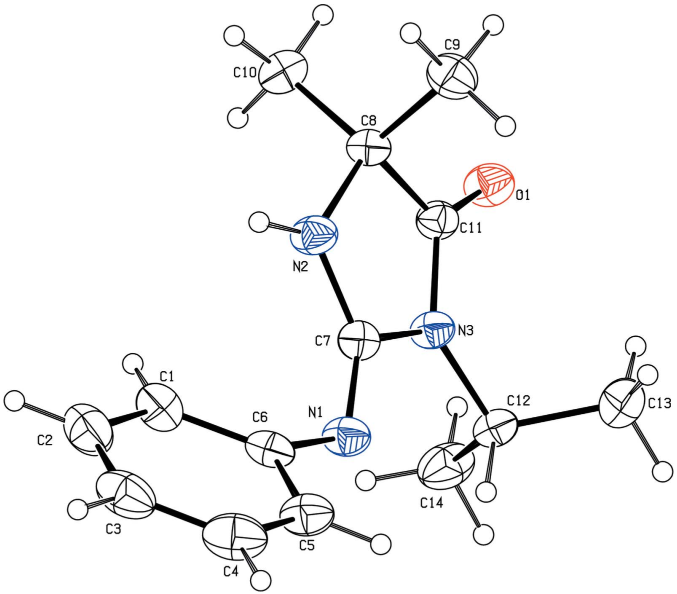


Figure 1
View of the molecule, showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are reprsented by spheres of arbitrary size.

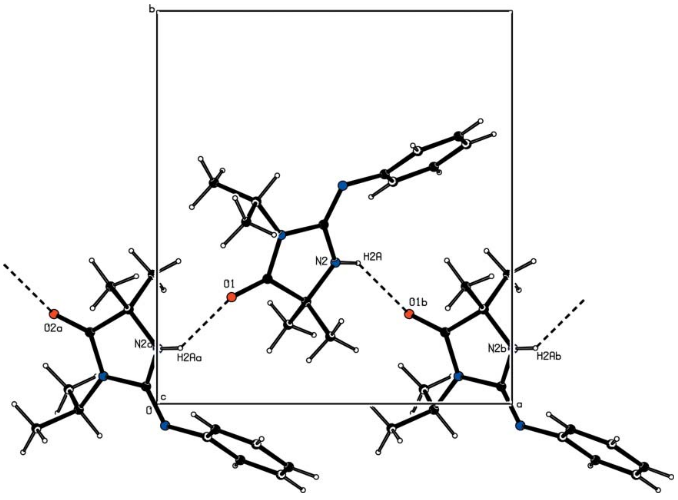


Figure 2
Hydrogen-bonding interactions forming a chain.

Crystal data

$C_{14}H_{19}N_3O$
$M_r = 245.32$
Orthorhombic, $P2_12_12_1$
$a = 10.2783$ (11) Å
$b = 11.4013$ (11) Å
$c = 11.5930$ (12) Å
$V = 1358.5$ (2) Å^3
$Z = 4$
$D_x = 1.199$ Mg m^{-3}

Mo $K\alpha$ radiation
Cell parameters from 2657 reflections
$\theta = 2.5$–22.9°
$\mu = 0.08$ mm^{-1}
$T = 292$ (2) K
Block, colorless
0.30 × 0.30 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
$T_{\min} = 0.977$, $T_{\max} = 0.985$
7376 measured reflections

1539 independent reflections
1406 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.029$
$\theta_{\max} = 26.0°$
$h = -12 \rightarrow 12$
$k = -14 \rightarrow 9$
$l = -12 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.103$
$S = 1.09$
1539 reflections
167 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.065P)^2 + 0.0483P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.18$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}

H atoms were placed in calculated positions and treated as riding atoms (C—H = 0.93–0.98 Å), with $U_{\rm iso}$ values set at 1.2 (CH) or 1.5 (CH_3) times $U_{\rm eq}$ of the parent atom. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-NT* (Siemens, 1995); software used to prepare material for publication: *SHELXTL-NT*.

The authors gratefully acknowledge financial support of this work by the National Natural Science Foundation of China (project No. 20102001).

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