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1-(2-Methylpropyl)-1*H*-imidazo[4,5-*c*]-quinolin-4-amine

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.115
Data-to-parameter ratio = 10.1

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

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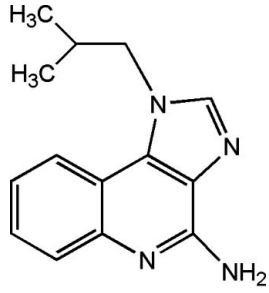
In the title compound, $C_{14}H_{16}N_4$, the imidazole ring is coplanar with the quinoline system. In the solid state, the molecules are linked by N—H···N hydrogen bonds which propagate in a chain parallel to the *a* axis.

Comment

The title compound, (I), exhibits wide-spectrum antiviral activity and is used topically to treat genital and anal warts. It is an immune response modifier (Miller *et al.*, 1999; Jappe & Gollnick, 1998). The X-ray crystallographic analysis of (I) shows that the imidazole ring is coplanar with the quinoline system (Fig. 1). As shown in Fig. 2, the molecules are linked by intermolecular N—H···N hydrogen bonds (Table 2). No π–π stacking is observed in the crystal structure. Selected torsion angles describing the molecular conformation are listed in Table 1.



(I)

Experimental

The title compound was synthesized according to Gerster (1985). Crystals appropriate for data collection were obtained by slow evaporation of an ethanol solution at room temperature.

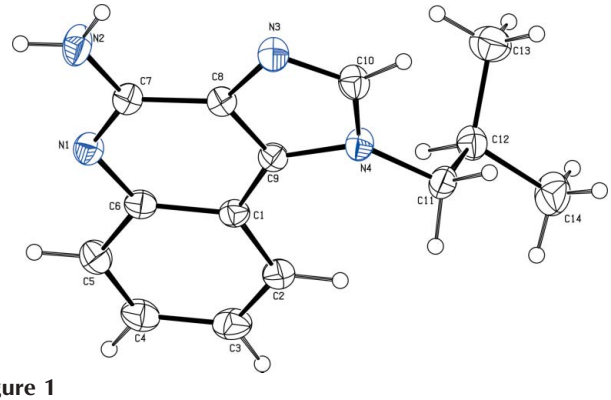


Figure 1
View of the molecule of (I), showing the atom-labeling scheme, with displacement ellipsoids drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

Crystal data

$C_{14}H_{16}N_4$
M_r = 240.31
Orthorhombic, $P2_12_12_1$
a = 8.1306 (9) Å
b = 9.7446 (11) Å
c = 15.7357 (18) Å
V = 1246.7 (2) Å^3
Z = 4
D_x = 1.280 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2290 reflections
θ = 2.5–24.4°
μ = 0.08 mm^{-1}
T = 292 (2) K
Block, colorless
0.34 × 0.20 × 0.18 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1997)
T_{min} = 0.973, T_{max} = 0.986
7920 measured reflections
1664 independent reflections
1419 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.5°
$h = -8 \rightarrow 10$
$k = -12 \rightarrow 11$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.115
S = 1.01
1664 reflections
165 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.069P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N3—C8	1.385 (3)	N1—C7	1.317 (3)
N2—C7	1.347 (3)	N4—C9	1.383 (3)
C10—N3—C8	103.48 (18)	N4—C11—C12	113.12 (19)
C10—N4—C9	105.95 (18)	N3—C10—N4	114.4 (2)
N1—C7—C8—N3	−179.5 (2)	C9—N4—C11—C12	72.9 (3)
C6—C1—C9—N4	179.4 (2)	C11—N4—C10—N3	177.0 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···N3^{i}	0.86	2.24	3.103 (3)	176
N2—H2B···N1^{ii}	0.86	2.33	3.125 (3)	153

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

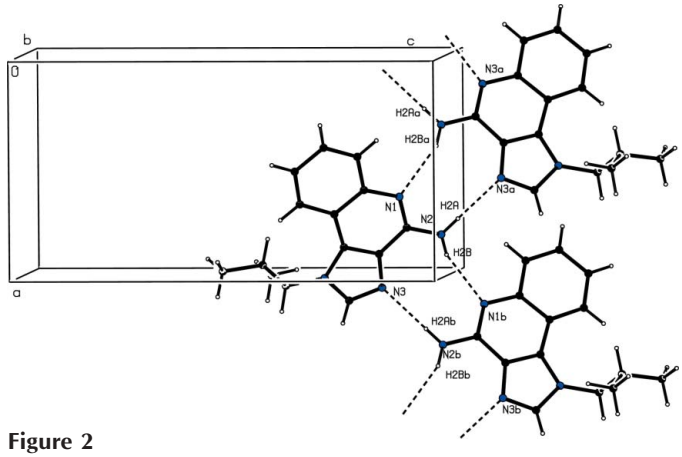


Figure 2
The intermolecular hydrogen bonding (dashed lines) in the crystal structure of (I).

H atoms were placed at calculated positions and refined as riding atoms (N—H = 0.86 Å and C—H = 0.93 and 0.98 Å), with U_{iso}(H) equal to 1.2 (CH) or 1.5 (OH and CH_3) times U_{eq}(parent atom). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); 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); software used to prepare material for publication: *SHELXTL*.

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