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3-Methyl-1-phenyl-4-[phenyl(8-quinolylamino)methylene]pyrazol-5(4*H*)-one

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.115
Data-to-parameter ratio = 13.1

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

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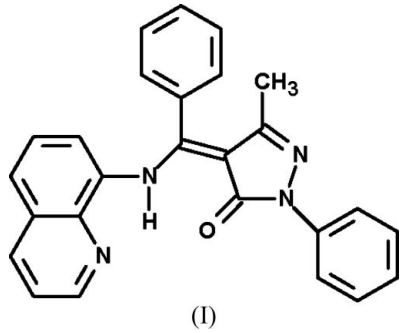
The title compound, $C_{26}H_{20}N_4O$, was synthesized by the reaction of 1-phenyl-3-methyl-4-benzoylpyrazol-5-one and 8-aminoquinoline. The molecule exists in the enamine–keto tautomeric form.

Comment

The title compound, (I), was prepared as part of our continuing study of pyrazolone derivatives which are well known for their potential applications in the areas of pharmaceuticals, agrochemicals, dyes, and pigments, and also as chelating agents and extracting agents. Moreover, they are capable of prototropic tautomerism (Akama & Tong, 1996; Eller & Holzer, 2004).



(I)

The molecule of compound (I) is not planar and possesses normal geometric parameters. The dihedral angles between the pyrazolone ring (N1/N2/C1–C3) plane and the phenyl (C4–C9 and C12–C17) and quinolyl ring planes (N4/C18–C26) are 40.8 (1), 108.2 (2) and 47.8 (1)°, respectively. The molecule exists in the enamine–keto tautomeric form in the crystalline state (Table 1 and Fig. 1), rather than the imine form as in 4-[(*Z*)-(benzylamino)phenylmethylene]-5-methyl-2-phenyl-2*H*-pyrazol-3-one (Jiang *et al.*, 2004). Similar tautomerism has also been observed in a pyrazolone–hydrazide compound (Sun *et al.*, 2006). In addition, the present compound also features an intramolecular hydrogen bond between the atoms N3 and O1 (Fig. 1), leading to the fact that atoms O1 and N3 are on the same side of the C2—C11 bond, which will be the potential bidentate *N*,*O*-chelate positions after deprotonation to form functional complexes as candidates with catalytic applications (Lu *et al.*, 2006). This is obviously different from the situation in 9-[ethoxy(8-quinolylamino)methyl]anthracene (Huang *et al.*, 2004), in which the intramolecular hydrogen bond involves the quinoline N atom [N3—H3···O1: N3—H3 = 0.86 Å, H3···O1 = 1.99 Å, N3···O1 = 2.714 (1) Å and N3—H3···O1 = 141°].

Experimental

A mixture of 1-phenyl-3-methyl-4-benzoylpyrazol-5-one (1 mmol) and 8-aminoquinoline (1 mmol) in anhydrous ethanol (30 ml) was refluxed for 3 h, and then cooled to room temperature. The precipitate was filtered off and dried. The crude product was recrystallized from ethanol. Yellow crystals were obtained in 78% yield. Analysis calculated for $C_{26}H_{20}N_4O$: C 77.21, H 4.98, N 13.85%; found: C 77.28, H 4.93, N 13.82%. A single crystal suitable for an X-ray structural analysis was obtained by slowly evaporating an ethanol solution at room temperature.

Crystal data

$C_{26}H_{20}N_4O$
M_r = 404.46
Monoclinic, $P2_1/n$
a = 7.3870 (10) Å
b = 26.563 (4) Å
c = 10.7360 (15) Å
β = 99.937 (2)°
V = 2075.0 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 273 (2) K
0.95 × 0.28 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.927, T_{max} = 0.992
10524 measured reflections
3657 independent reflections
3227 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.115
S = 1.00
3657 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.2418 (15)	C1—C2	1.4454 (17)
N2—C3	1.3060 (16)	C2—C11	1.3877 (17)
N3—C11	1.3396 (16)	C2—C3	1.4428 (18)
N3—C18	1.4154 (16)	C11—C12	1.4829 (18)
C11—N3—C18	129.62 (11)	N3—C11—C2	118.35 (11)
O1—C1—C2	129.92 (11)	N3—C11—C12	119.53 (11)
C11—C2—C3	132.31 (11)	C2—C11—C12	122.12 (11)
C11—C2—C1	122.29 (11)	N3—C18—C26	115.82 (11)

All H atoms were initially located in a difference Fourier map. The methyl and methylene H atoms were then constrained to an ideal geometry, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). The amino H atom was treated as a riding atom, with N—H = 0.86 Å and U_{iso}(H) = 1.2U_{eq}(N). All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

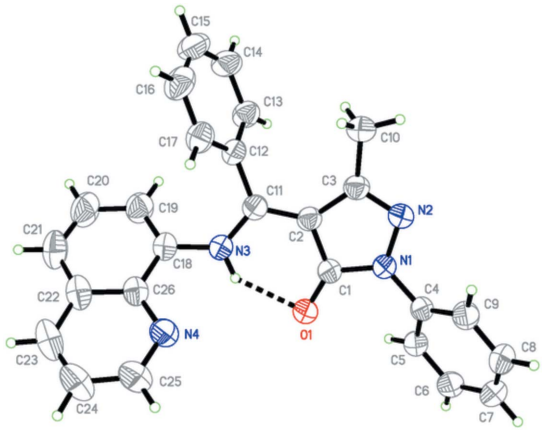


Figure 1
The molecular stucture of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius. The dashed line indicates a hydrogen bond.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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