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1,5-Dimethyl-2-phenyl-4-[(1*E*)-(2-quinolyl)-methylideneamino]-1*H*-pyrazol-3(2*H*)-one

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.059
wR factor = 0.165
Data-to-parameter ratio = 15.5

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

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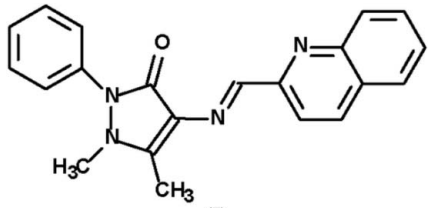
The title compound, $C_{21}H_{18}N_4O$, was synthesized by condensation of quinoline-2-carbaldehyde and 4-aminoantipyrine. The mean planes of the pyrazole and phenyl rings make a dihedral angle of 55.7 (3)°. The crystal packing is stabilized by weak intermolecular C—H···O hydrogen bonds and π–π interactions.

Comment

Schiff bases often demonstrate antitumor, antimicrobial and antiviral properties (Siddiqui *et al.*, 2006). Antipyrine (2,3-dimethyl-1-phenylpyrazol-5-one) and its derivatives exhibit a wide range of biological activities (Yadav *et al.*, 2003). Antipyrine is also a multifunctional marker drug extensively used in the study of hepatic oxidative metabolism (Marques *et al.*, 2002). In a continuation of our studies of antipyrine Schiff base derivatives, we report the synthesis and crystal structure of the title compound, (I) (Fig. 1).



(I)

The bond lengths and angles in (I) are normal (Allen *et al.*, 1987). The mean planes of the pyrazole and phenyl rings make a dihedral angle of 55.7 (3)°. The molecule adopts an *E* configuration about the central C=N double bond, as observed in 4-(4-chlorobenzylideneamino)-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Sun *et al.*, 2006) and 4-[(1*E*)-(2-hydroxy-5-nitrophenyl)methyleneamino]-1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-one (Chen & Huang, 2007), but not in the related antipyrine Schiff base analogues reported by Sun *et al.* (2007).

The short $Cg1\cdots Cg2^{ii}$ distance [3.629 (3) Å; *Cg*1 and *Cg*2 are the centroids of rings C16–C21 and N1/N2/C1–C3, respectively; symmetry code: (ii) $2-x, 2-y, -z$] indicates the presence of π–π interactions, which contribute to the crystal-packing stabilization, along with weak intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

A mixture of 4-aminoantipyrine (1 mmol) and quinoline-2-carbaldehyde (1 mmol) in anhydrous ethanol (30 ml) was refluxed for 2 h, and then cooled to room temperature. The precipitate was filtered off

and dried. The crude product was recrystallized from ethanol in 73% yield. Single crystals of X-ray quality were obtained by slow evaporation of an ethanol solution at room temperature.

Crystal data

$C_{21}H_{18}N_4O$
M_r = 342.39
Monoclinic, $P2_1/n$
a = 12.935 (3) Å
b = 7.1220 (14) Å
c = 20.465 (4) Å
β = 105.88 (3)°
V = 1813.4 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
0.20 × 0.18 × 0.17 mm

Data collection

Rigaku R-AXIS-IV diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.984, T_{max} = 0.987
5958 measured reflections
3655 independent reflections
2472 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.165
S = 1.06
3655 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19A···O1^{i}	0.93	2.44	3.318 (3)	159

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

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

Data collection: *RAXIS* (Rigaku, 1996); cell refinement: *RAXIS*; data reduction: *RAXIS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *TEXSAN* (Molecular Structure Corporation, 1999); software used to prepare material for publication: *TEXSAN*.

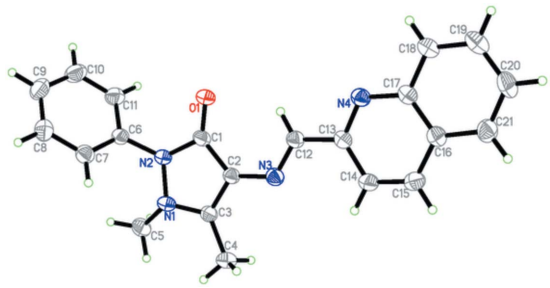


Figure 1
The molecular structure of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radius.

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References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Chen, D.-B. & Huang, L. (2007). *Acta Cryst.* E**63**, o36–o37.
Marques, M. P., Takayanagui, O. M. & Lanchote, V. L. (2002). *Braz. J. Med. Biol. Res.* **35**, 261–269.
Molecular Structure Corporation (1999). *TEXSAN*. Version 1.10. MSC, The Woodlands, Texas, USA.
Rigaku (1996). *RAXIS*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siddiqui, H. L., Iqbal, A., Ahmad, S. & Weaver, G. W. (2006). *Molecules*, **11**, 206–211.
Sun, Y. F., Zheng, Z. B., Wang, H. C. & Gao, H. Y. (2007). *Anal. Sci. X*, **23**, x11–12.
Sun, Y.-X., Zhang, R., Jin, Q.-M., Zhi, X.-J. & Lü, X.-M. (2006). *Acta Cryst.* C**62**, o467–o469.
Yadav, P. N., Demertzis, M. A., Kovala-Demertzi, D., Skoulika, S. & West, D. X. (2003). *Inorg. Chim. Acta*, **349**, 30–36.