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1,5-Dimethy-4-[(2-nitrobenzylidene)amino]-2-phenyl-1*H*-pyrazol-3(4*H*)-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.087
Data-to-parameter ratio = 9.7

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

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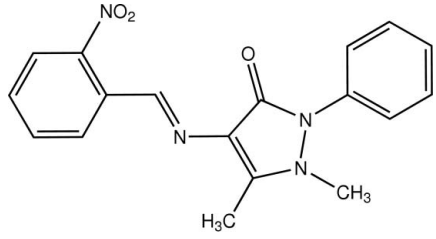
The title compound, $C_{18}H_{16}N_4O_3$, has been synthesized by the reaction of 2-nitrobenzaldehyde and 4-aminoantipyrine. The molecule adopts an *E* configuration about the central C=N double bond.

Comment

The roles of antipyrine and antipyridine derivatives in biological processes have become a topic of study in recent years (Carlton *et al.*, 1995; Coolen *et al.*, 1999; Jiang *et al.*, 2000). The title compound, (I), is a new antipyrine Schiff base compound prepared in our laboratory. We present its structure here.



(I)

The molecular structure of (I) is shown in Fig. 1. The C10=N3 bond length (Table 1) shows the character of a Schiff base. The molecule adopts an *E* configuration about the central C10=N3 double bond. The pyrazole is nearly coplanar with the C11-containing benzene ring [dihedral angle = 14.51 (14)°], but is tilted with respect to the C1-containing benzene ring [dihedral angle = 54.69 (14)°].

Experimental

2-Nitrobenzaldehyde (0.1 mmol, 15.1 mg) and 4-aminoantipyrine (0.1 mmol, 20.3 mg) were dissolved in methanol (10 ml). The solution was stirred for 30 min at room temperature to give a clear yellow solution. Single crystals of (I) were obtained from the filtrate.

Crystal data

$C_{18}H_{16}N_4O_3$
M_r = 336.35
Orthorhombic, $P2_12_12_1$
a = 6.886 (1) Å
b = 13.382 (1) Å
c = 17.872 (2) Å
V = 1646.9 (3) Å^3
Z = 4
D_x = 1.357 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 (2) K
Rod, yellow
0.58 × 0.26 × 0.22 mm

Data collection

Siemens P4 diffractometer
ω scans
Absorption correction: none
2318 measured reflections
2221 independent reflections
1272 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 27.7°
3 standard reflections
every 97 reflections
intensity decay: 5.3%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.040$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.087$	$\Delta\rho_{max} = 0.15$ e Å^{-3}
$S = 0.84$	$\Delta\rho_{min} = -0.14$ e Å^{-3}
2221 reflections	Extinction correction: *SHELXL97*
229 parameters	Extinction coefficient: 0.0229 (18)
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

O1—C7	1.228 (3)	N2—C9	1.356 (3)
N1—N2	1.397 (3)	N2—C17	1.462 (3)
N1—C7	1.408 (3)	N3—C10	1.279 (3)
N1—C6	1.433 (3)		

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å, and the torsion angles refined to fit the electron density, with U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.93 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

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

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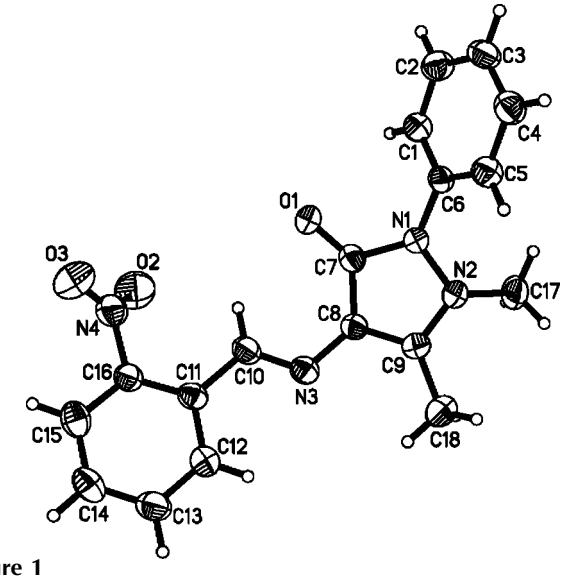

Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

References

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