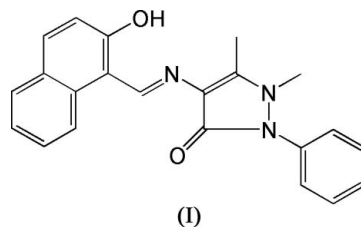


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## Key indicators

Single-crystal X-ray study  
*T* = 298 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$   
*R* factor = 0.069  
*wR* factor = 0.180  
Data-to-parameter ratio = 16.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.4-[[*(2-Hydroxy-1-naphthyl)methylidene*]-  
1,5-dimethyl-2-phenyl-1*H*-pyrazol-3(2*H*)-oneThe title compound,  $\text{C}_{22}\text{H}_{19}\text{N}_3\text{O}_2$ , is a Schiff base compound  
derived from 4-aminoantipyrene and 2-hydroxy-1-naphthalde-  
hyde. As expected, the two crystallographically independent  
molecules adopt *trans* configurations about the central  $\text{C}=\text{N}$   
bonds.Received 3 March 2006  
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## Comment

Antipyrene and its derivatives exhibit a wide range of biolo-  
gical activities and applications (Yadav *et al.*, 2003; Ismail,  
2000; Abd El Rehim *et al.*, 2001). The structures of antipyrene  
derivatives have also been investigated (Li & Zhang, 2004,  
2005; Zhang & Li, 2005; Liang *et al.*, 2002; You *et al.*, 2003,  
2004). As an extension of such work on the structural char-  
acterization of antipyrene derivatives, a new compound, (I), is  
reported here.

The asymmetric unit of (I) consists of two independent molecules (Fig. 1). In both of these, the bond lengths and angles are in normal ranges, close to those observed in similar antipyrene Schiff bases cited above. The dihedral angle between the N2/N3/C12/C13/C16 pyrazoline ring and the C17–C22 benzene ring is  $64.6(3)^\circ$  and that between the N5/N6/C34/C35/C38 pyrazoline ring and the C39–C44 benzene ring is  $65.4(3)^\circ$ . Atom O2 deviates from the pyrazoline mean plane by  $0.166(4) \text{ \AA}$ , whereas atoms C14 and C15 deviate from it, on the other side, by  $0.123(5)$  and  $0.456(5) \text{ \AA}$ , respectively. Atom O4 deviates from the other pyrazoline mean plane by  $0.091(4) \text{ \AA}$ , whereas atoms C36 and C37 deviate from it, on the opposite side, by  $0.123(5)$  and  $0.419(5) \text{ \AA}$ , respectively. As a result of conjugation through the imino double bonds, the pyrazoline and the naphthyl ring systems in both molecules are nearly coplanar; the dihedral angle between the N2/N3/C12/C13/C16 pyrazoline ring and the C1–C10 naphthyl ring system is  $9.4(4)^\circ$  [mean deviation from the combined mean plane is  $0.074(5) \text{ \AA}$ ] and that between the N5/N6/C34/C35/C38 pyrazoline ring and the C23–C32 naphthyl ring system is  $8.4(4)^\circ$  [mean deviation from the combined mean plane is  $0.068(5) \text{ \AA}$ ]. As expected, the two molecules adopt *trans* configurations about the  $\text{C}11=\text{N}1$  and  $\text{C}33=\text{N}4$  bonds. There are no short contacts among the molecules.

## Experimental

A mixture of 2-hydroxy-1-naphthaldehyde (0.1 mmol, 172.2 mg) and 4-aminoantipyrine (0.1 mmol, 20.3 mg) was dissolved in MeOH (20 ml). The mixture was stirred for about 10 min at room temperature to give a clear yellow solution. After allowing the solution to stand in air for 7 d, yellow block-shaped crystals were formed. Analysis found: C 73.72, H 5.50, N 11.83%; calculated for  $C_{22}H_{19}N_3O_2$ : C 73.93, H 5.36, N 11.76%.

### Crystal data

$C_{22}H_{19}N_3O_2$	Mo $K\alpha$ radiation
$M_r = 357.40$	Cell parameters from 2824 reflections
Orthorhombic, $Pna2_1$	$\theta = 2.3\text{--}24.9^\circ$
$a = 11.713$ (1) Å	$\mu = 0.08$ mm $^{-1}$
$b = 14.951$ (1) Å	$T = 298$ (2) K
$c = 21.877$ (2) Å	Block, yellow
$V = 3831.1$ (5) Å $^3$	$0.30 \times 0.17 \times 0.10$ mm
$Z = 8$	
$D_x = 1.239$ Mg m $^{-3}$	

### Data collection

Bruker SMART CCD area-detector diffractometer	7941 independent reflections
$\omega$ scans	4828 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.058$
$T_{\text{min}} = 0.976$ , $T_{\text{max}} = 0.992$	$\theta_{\text{max}} = 26.5^\circ$
29274 measured reflections	$h = -14 \rightarrow 14$
	$k = -18 \rightarrow 18$
	$l = -27 \rightarrow 27$

### Refinement

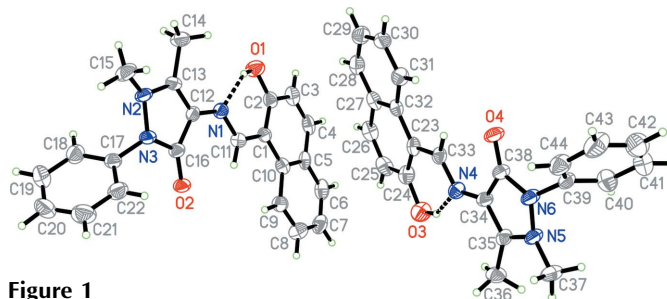
Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.069$	$w = 1/[\sigma^2(F_o^2) + (0.0909P)^2]$
$wR(F^2) = 0.180$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{\text{max}} < 0.001$
7941 reflections	$\Delta\rho_{\text{max}} = 0.32$ e Å $^{-3}$
492 parameters	$\Delta\rho_{\text{min}} = -0.17$ e Å $^{-3}$

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3 $\cdots$ N4	0.82	1.82	2.541 (4)	147
O1—H1 $\cdots$ N1	0.82	1.80	2.523 (4)	146

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å, O—H distances of 0.82 Å and with  $U_{\text{iso}}(\text{H}) = 1.2$



**Figure 1**

The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The dashed lines indicate hydrogen bonds.

or  $1.5U_{\text{eq}}(\text{C},\text{O})$ . The structure contains solvent-accessible voids of 55 Å $^3$ , which might accommodate a disordered water molecule. In the absence of significant anomalous scattering effects, 3860 Friedel pairs were merged before the final refinement.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997a); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997a); molecular graphics: SHELXTL (Sheldrick, 1997b); software used to prepare material for publication: SHELXTL.

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