

## 1-[(4-Acetylphenylamino)methylene]-naphthalen-2(1H)-one

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## Key indicators

Single-crystal X-ray study

$T = 293\text{ K}$

Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$

$R$  factor = 0.036

$wR$  factor = 0.089

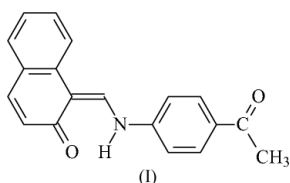
Data-to-parameter ratio = 11.1

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

The molecule of the title compound,  $\text{C}_{19}\text{H}_{15}\text{NO}_2$ , is nearly planar and adopts the keto–amine tautomeric form, with a strong intramolecular  $\text{N}-\text{H}\cdots\text{O}$  [2.5383 (17) Å] hydrogen bond.

## Comment

Schiff bases have been widely used as ligands in the field of coordination chemistry (Calligaris & Randaccio, 1987). Schiff base compounds show photochromism and thermochromism in the solid state by proton transfer from the hydroxyl O atom to the imine N atom (Cohen *et al.*, 1964), *i.e.* phenol–imine keto–amine tautomerism. In solution, this tautomerism, which depends on the formation of intramolecular hydrogen bonds, is possible (Filarowski & Koll, 1998; Yıldız *et al.*, 1998; Nazır *et al.*, 2000; Deziembowska *et al.*, 2001; Ünver *et al.*, 2001). In the solid state, the keto–amine tautomer is dominant in naphthaldimine (Hökelek *et al.*, 2002; Ünver *et al.*, 2002; Odabaşoğlu *et al.*, 2004), while the phenol–imine tautomer is found in salicylaldimine Schiff bases (Kaitner & Pavlovic, 1996; Yıldız *et al.*, 1998; Elmalı *et al.*, 1998; Karadayı *et al.*, 2003; Odabaşoğlu *et al.*, 2004; Yüce *et al.*, 2004).

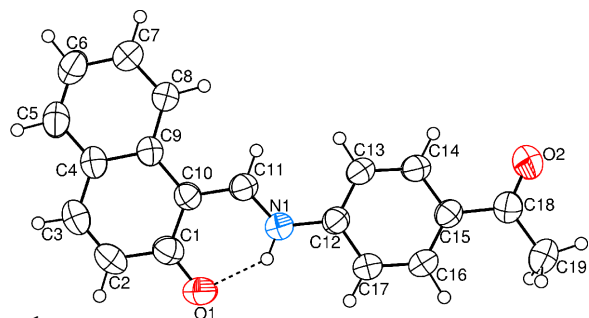


The title compound, (I), adopts the keto–imine tautomeric form, with a strong intramolecular  $\text{N1}-\text{H1}\cdots\text{O1}$  hydrogen bond (Fig. 1). The rather short  $\text{C1}-\text{O1}$ ,  $\text{C18}-\text{O2}$  and  $\text{C2}-\text{C3}$ ,  $\text{C5}-\text{C6}$ ,  $\text{C7}-\text{C8}$  bonds can be considered as  $\text{C}=\text{O}$  and  $\text{C}=\text{C}$  double bonds, respectively. This suggests the presence of a significant quinoidal effect. A similar effect was observed in 1-[*N*-(*p*-hydroxyphenyl)aminomethylidene]naphthalen-2(1H)-one propan-1-ol hemisolvate [ $\text{C}=\text{O} = 1.292$  (2) and 1.295 Å; Odabaşoğlu *et al.*, 2004] and *N*-*n*-propyl-2-oxo-1-naphthylidenemethylamine [ $\text{C}=\text{O} = 1.277$  (2) Å; Kaitner & Pavlovic, 1996].

The study of Schiff bases has led to the proposal that molecules exhibiting thermochromism are planar, while those exhibiting photochromism are non-planar. Molecule (I) is nearly planar; the dihedral angle between the rings *A* (atoms  $\text{C12}-\text{C17}$ ) and *B* (atoms  $\text{C1}-\text{C10}$ ) is 10.98 (4)°.

## Experimental

The title compound, (I), was prepared as described in the literature (Odabaşoğlu *et al.*, 2004), using 4-acetylaniline and 2-hydroxy-1-



**Figure 1**  
A view of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bond.

naphthol as starting materials. Crystals of (I) were obtained by slow evaporation of an acetone solution (yield 92%, m.p. 479–481 K).

#### Crystal data

$C_{19}H_{15}NO_2$	$D_x = 1.333 \text{ Mg m}^{-3}$
$M_r = 289.32$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 11906 reflections
$a = 6.7815 (4) \text{ \AA}$	$\theta = 2.0\text{--}28.4^\circ$
$b = 14.0948 (12) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$c = 15.0855 (10) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\beta = 90.050 (5)^\circ$	Prism, orange
$V = 1441.93 (18) \text{ \AA}^3$	$0.38 \times 0.31 \times 0.28 \text{ mm}$
$Z = 4$	

#### Data collection

Stoe IPDS-2 diffractometer  
 $\omega$  scans  
 Absorption correction: none  
 20326 measured reflections  
 2839 independent reflections  
 1731 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$   
 $\theta_{\text{max}} = 26.0^\circ$   
 $h = -8 \rightarrow 8$   
 $k = -17 \rightarrow 17$   
 $l = -18 \rightarrow 18$

#### Refinement

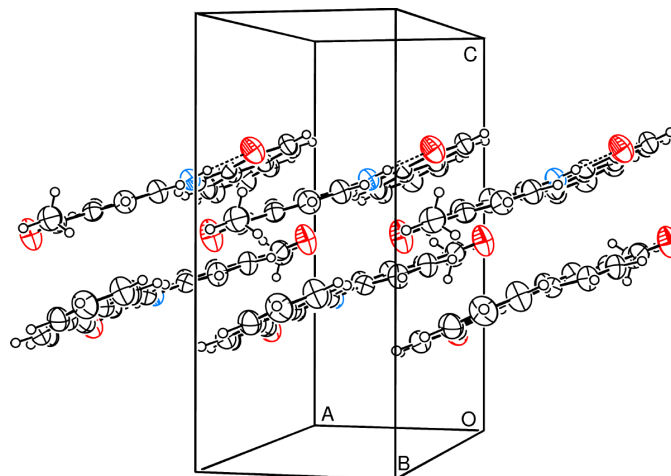
Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.089$   
 $S = 0.85$   
 2839 reflections  
 255 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0571P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.10 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

C1—O1	1.2822 (17)	C8—C9	1.402 (2)
C1—C10	1.4305 (19)	C9—C10	1.4508 (19)
C1—C2	1.436 (2)	C10—C11	1.3988 (19)
C2—C3	1.336 (2)	C11—N1	1.3161 (17)
C3—C4	1.425 (2)	C12—N1	1.4056 (17)
C4—C5	1.401 (2)	C18—O2	1.2141 (18)
C5—C6	1.357 (2)	C18—C19	1.499 (2)
C6—C7	1.390 (2)	N1—H1	0.86
C7—C8	1.369 (2)		
O1—C1—C10	122.07 (13)	N1—C11—H8	118.2 (8)
O1—C1—C2	119.74 (14)	C13—C12—N1	122.46 (12)
C11—C10—C1	119.14 (13)	C17—C12—N1	118.01 (13)
C11—C10—C9	120.95 (12)	C11—N1—C12	126.33 (12)
N1—C11—C10	123.08 (14)		
O1—C1—C2—C3	−179.34 (15)	N1—C12—C17—C16	178.46 (13)
C1—C10—C11—N1	0.9 (2)	C10—C11—N1—C12	178.81 (13)
C9—C10—C11—N1	178.75 (13)	C13—C12—N1—C11	−11.0 (2)
N1—C12—C13—C14	−178.88 (13)	C17—C12—N1—C11	170.54 (13)



**Figure 2**  
A view of the packing in (I).

**Table 2**

Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
N1—H1 $\cdots$ O1	0.86	1.84	2.5383 (16)	137

All H atoms were found in difference density maps. H1 attached to N1 was refined as riding, with  $N\text{—}H = 0.86 \text{ \AA}$  and  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(N)$ . H atoms attached to carbon were refined freely [ $C\text{—}H = 0.92 (2)\text{--}0.99 (2) \text{ \AA}$ ].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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