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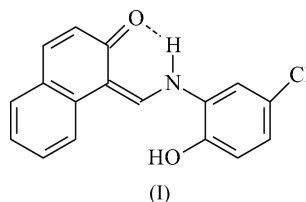
## Key indicators

Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$   
*R* factor = 0.063  
*wR* factor = 0.112  
Data-to-parameter ratio = 13.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.1-[(5-Chloro-2-hydroxyphenylamino)methylene]-  
naphthalen-2(1*H*)-one

The molecule of the title compound,  $\text{C}_{17}\text{H}_{12}\text{ClNO}_2$ , is not exactly planar, and adopts the keto–amine tautomeric form. There is an intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bond, and intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds link the molecules into a three-dimensional network.

## Comment

Although Schiff bases have been widely used as ligands in the formation of transition metal complexes and structurally characterized, a relatively small number of free Schiff bases have been similarly characterized (Calligaris & Randaccio, 1987). Schiff bases play an important role in many fields of chemistry and biochemistry (Lozier *et al.*, 1975; Garnovskii *et al.*, 1993). Two characteristic properties of Schiff bases are photochromism and thermochromism (Cohen *et al.*, 1964; Moustakali-Mavridis *et al.*, 1978). These properties are caused by proton transfer from the hydroxyl O atom to the imine N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994). Schiff bases display two possible tautomeric forms, *viz.* the phenol-imine and keto-amine forms. In the solid state, the keto-amine tautomer has been found in naphthaldimine Schiff bases (Hökelek *et al.*, 2000; Ünver *et al.*, 2001; Odabaşoğlu *et al.*, 2003; Özek *et al.*, 2004), whereas the phenol-imine tautomer exists in salicylaldimine Schiff bases (Kaitner & Pavlovic, 1996; Yıldız *et al.*, 1998).



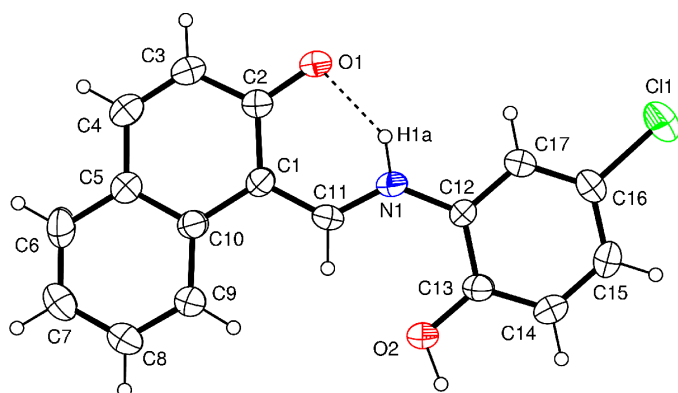
In the title compound, (I), the keto-amine tautomer is favoured over the phenol-imine form (Fig. 1 and Table 1), and there is a strong intramolecular hydrogen bond,  $\text{N1}-\text{H1a}\cdots\text{O1}$ . The sum of the van der Waals radii of oxygen and nitrogen is  $3.07 \text{ \AA}$  (Bondi, 1964), and the intramolecular hydrogen bond in (I) is much shorter than this, *viz.*  $2.590(4) \text{ \AA}$ .

The somewhat short  $\text{C2}-\text{O1}$  and  $\text{C1}-\text{C11}$  bonds can be considered as  $\text{C}=\text{O}$  and  $\text{C}=\text{C}$  double bonds, respectively. This fact, together with the very short  $\text{C3}-\text{C4}$  bond, suggests the presence of a significant quinoidal effect. A similar effect was observed for 1-[(3-hydroxypyridin-2-ylamino)methylene]-1*H*-naphthalen-2-one [ $\text{C}=\text{O}$   $1.276(2) \text{ \AA}$ ; Özek *et al.*, 2004], 1-[*N*-(*p*-hydroxyphenyl)aminomethylidene]naphthalen-2(1*H*)-one propan-1-ol hemisolvate [ $\text{C}=\text{O}$   $1.292(2) \text{ \AA}$  and

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**Figure 1**

An ORTEP view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. The intramolecular hydrogen bond is indicated by the dashed line.

1.295 (2) Å; Odabaşoğlu *et al.*, 2004] and *N-n*-propyl-2-oxo-1-naphthylidenemethylamine [C=O 1.277 (2) Å; Kaitner & Pavlovic, 1996]. The keto-amine form is also dominant in *N*-( $\alpha$ -naphthyl)-2-oxo-1-naphthalimine [C=O 1.287 (5) Å; Gavranic *et al.*, 1996].

The title molecule is not exactly planar, with a dihedral angle of 10.20 (15)° between ring A (atoms C12–C17) and ring B (atoms C1–C5/C10). The hydrogen-bonded ring (N1, H1a, O1, C2, C1, C11) is almost planar. The C11–N1 bond length and C11–N1–C12 bond angle are 1.313 (4) Å and 130.6 (3)°, respectively, compared with 1.3237 (19) Å and 125.96 (16)° in 1-[(3-hydroxypyridin-2-ylamino)methylene]-1*H*-naphthalen-2-one (Özek *et al.*, 2004).

The molecules are linked by strong intermolecular O–H···O hydrogen bonds (Table 2) into a three-dimensional network.

## Experimental

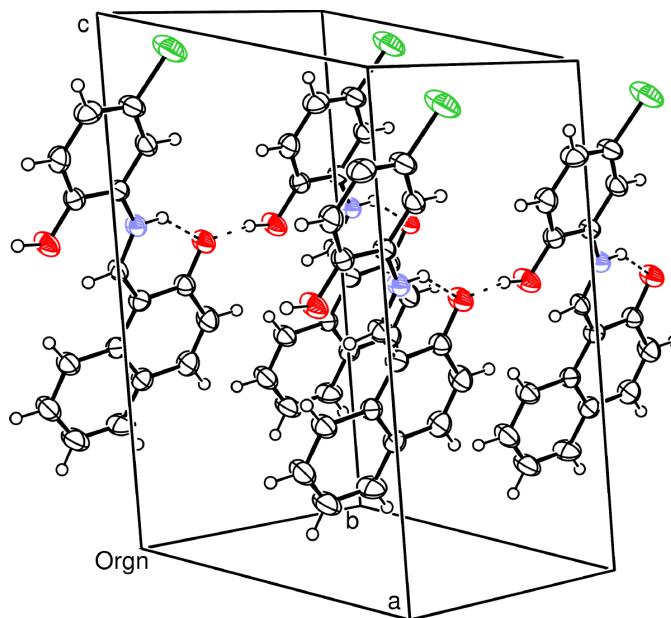
The title compound, (I), was prepared as described in the literature (Odabaşoğlu *et al.*, 2003), using 2-amino-4-chlorophenol and 2-hydroxy-1-naphthol as starting materials. Crystals of (I) were obtained by slow evaporation of a THF solution (yield 87%, m.p. 545–546 K).

### Crystal data

C <sub>17</sub> H <sub>12</sub> ClNO <sub>2</sub>	Z = 2
M <sub>r</sub> = 297.73	D <sub>x</sub> = 1.470 Mg m <sup>-3</sup>
Triclinic, P $\bar{1}$	Mo K $\alpha$ radiation
a = 7.293 (5) Å	Cell parameters from 4334 reflections
b = 7.865 (5) Å	$\theta$ = 2.9–28.8°
c = 13.628 (5) Å	$\mu$ = 0.29 mm <sup>-1</sup>
$\alpha$ = 88.973 (5)°	T = 293 (2) K
$\beta$ = 74.668 (5)°	Plate, orange
$\gamma$ = 63.876 (5)°	0.16 × 0.12 × 0.04 mm
V = 672.5 (7) Å <sup>3</sup>	

### Data collection

Stoe IPDS 2 diffractometer	2638 independent reflections
$\omega$ scans	1319 reflections with $I > 2\sigma(I)$
Absorption correction: by integration (X-RED32; Stoe & Cie, 2002)	$R_{\text{int}} = 0.123$
$T_{\text{min}} = 0.951$ , $T_{\text{max}} = 0.990$	$\theta_{\text{max}} = 26.0^\circ$
9652 measured reflections	$h = -8 \rightarrow 8$
	$k = -9 \rightarrow 9$
	$l = -16 \rightarrow 16$



**Figure 2**

An ORTEP packing diagram. Dashed lines indicate intra- and intermolecular hydrogen bonds.

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.063$   
 $wR(F^2) = 0.112$   
 $S = 0.94$   
 2638 reflections  
 198 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0318P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.19 \text{ e } \text{Å}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.18 \text{ e } \text{Å}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

C1–C11	1.388 (5)	C4–C5	1.422 (5)
C1–C2	1.426 (5)	C5–C10	1.412 (5)
C1–C10	1.454 (4)	C11–N1	1.313 (4)
C2–O1	1.291 (4)	C12–N1	1.401 (4)
C2–C3	1.419 (5)	N1–H1a	0.88 (4)
C3–C4	1.349 (5)		
C11–C1–C2	120.1 (3)	N1–C11–C1	124.9 (3)
C11–C1–C10	120.1 (3)	C17–C12–N1	116.7 (3)
O1–C2–C3	120.7 (3)	C13–C12–N1	124.0 (3)
O1–C2–C1	121.4 (3)	C11–N1–C12	130.6 (3)
C11–C1–C2–O1	−7.7 (6)	C10–C1–C11–N1	−178.9 (4)
C2–C1–C11–N1	2.1 (6)	C1–C11–N1–C12	−178.6 (4)

**Table 2**

Hydrogen-bonding geometry (Å, °).

D–H···A	D–H	H···A	D···A	D–H···A
N1–H1a···O1	0.88 (4)	1.82 (4)	2.590 (4)	144 (3)
O2–H2a···O1 <sup>i</sup>	0.96 (5)	1.61 (5)	2.557 (4)	166 (4)

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

The H atoms attached to N and O were refined freely. Other H atoms were positioned geometrically (C–H = 0.93 Å) and refined using a riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$ .

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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