

(E)-1-[(2-Chloro-4-nitrophenylimino)-methyl]naphthalen-2-ol

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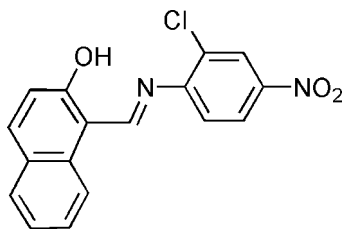
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.009$ Å; R factor = 0.080; wR factor = 0.185; data-to-parameter ratio = 12.0.

In the title compound, $\text{C}_{17}\text{H}_{11}\text{ClN}_2\text{O}_3$, an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond influences the molecular conformation; the naphthol system and the substituted benzene ring form a dihedral angle of 3.5 (1)°. In the crystal, weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds link molecules into chains in the [010] direction. The crystal packing exhibits $\pi-\pi$ interactions between the aromatic rings from the neighbouring molecules, with a centroid-centroid distance of 3.566 (7) Å.

Related literature

For general background to Schiff bases, see: Caligaris *et al.* (1972); Salman *et al.* (1990); Popovic *et al.* (2001); Garnovskii *et al.* (1993); Pyrz *et al.* (1985). For related structures, see: Burgess *et al.* (1999); Gayathri *et al.* (2007).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{11}\text{ClN}_2\text{O}_3$
 $M_r = 326.73$
Monoclinic, $P2_1/c$
 $a = 7.0530$ (8) Å

$b = 12.8699$ (13) Å
 $c = 15.7701$ (17) Å
 $\beta = 98.180$ (1)°
 $V = 1416.9$ (3) Å³

$Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.29$ mm⁻¹

$T = 298$ K
 $0.38 \times 0.13 \times 0.10$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2007)
 $T_{\min} = 0.899$, $T_{\max} = 0.972$

7115 measured reflections
2506 independent reflections
826 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.195$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.080$
 $wR(F^2) = 0.185$
 $S = 0.92$
2506 reflections

208 parameters
H-atom parameters constrained
 $\Delta\rho_{\max} = 0.30$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}$	0.82	1.81	2.547 (5)	149
$\text{C8}-\text{H8}\cdots\text{O3}^i$	0.93	2.50	3.392 (5)	160

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{7}{2}$.

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL and publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5095).

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supplementary materials

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(E)-1-[(2-Chloro-4-nitrophenylimino)methyl]naphthalen-2-ol

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Comment

Schiff base ligands play a vital role in coordination chemistry due to their metal binding ability (Garnovskii *et al.*, 1993). In addition, Schiff bases and their metal complexes have wide applications in biological systems (Pyrz *et al.*, 1985). 2-Hydroxy Schiff bases are formed by reactions of salicylaldehyde and 2-hydroxy-1-naphthaldehyde with various amines (Caligaris *et al.*, 1972). In contrast to salicylaldimine derivatives, the Schiff bases of 2-hydroxy-1-naphthaldehyde have been rarely investigated (Salman *et al.*, 1990; Popovic *et al.*, 2001). Herewith we present the title compound (I), derived from 2-hydroxy-1-naphthaldehyde.

In (I) (Fig. 1), the bond lengths and angles are normal and comparable with those observed for unsubstituted analogues (Burgess *et al.*, 1999; Gayathri *et al.*, 2007). Due to intramolecular O—H \cdots N hydrogen bond (Table 1), the C—N=C—C torsion angle (between the phenol and benzene rings) is close to 180° with the value of 178.4 (7)°. In the crystal structure, weak intermolecular C—H \cdots O hydrogen bonds (Table 1) link the molecules into chains in [010]. The crystal packing exhibits π - π interactions between the aromatic rings from the neighbouring molecules with centroid-centroid distance of 3.566 (7) Å.

Experimental

20 ml of methanol, 2-hydroxy-1-naphthaldehyde (0.172 g, 1 mmol), 2-chloro-4-nitrobenzenamine (0.172 g, 1 mmol) and four drops of acetic acid were added to a 50 ml round bottom flask with a magnetic stir bar. The solution was refluxed for 1.5 h until it was a bright orange color. The solution was then gravity filtered hot and allowed to slowly cool, yielding 0.268 g (78% yield) of bright orange-yellow needle-like crystals.

Refinement

H atoms were placed in idealized positions (C—H 0.95 - 0.98 Å, O—H 0.82 Å), and thereafter treated as riding, with U_{iso} (H) = 1.2-1.5 U_{eq} of the parent atom. In view of poor quality of the single-crystal sample selected for data collection (though it was the best one), the relatively high values of R_{int} and $R(F^2)$ were obtained.

Figures

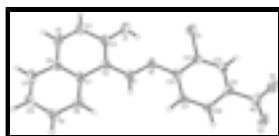


Fig. 1. The molecular structure of (I) with displacement ellipsoids shown at 30% probability level.

(E)-1-[(2-Chloro-4-nitrophenylimino)methyl]naphthalen-2-ol

Crystal data

$C_{17}H_{11}ClN_2O_3$	$F(000) = 672$
$M_r = 326.73$	$D_x = 1.532 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.0530 (8) \text{ \AA}$	Cell parameters from 381 reflections
$b = 12.8699 (13) \text{ \AA}$	$\theta = 2.6\text{--}17.6^\circ$
$c = 15.7701 (17) \text{ \AA}$	$\mu = 0.29 \text{ mm}^{-1}$
$\beta = 98.180 (1)^\circ$	$T = 298 \text{ K}$
$V = 1416.9 (3) \text{ \AA}^3$	Needle-like, orange
$Z = 4$	$0.38 \times 0.13 \times 0.10 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer	2506 independent reflections
Radiation source: fine-focus sealed tube graphite	826 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.195$
Absorption correction: multi-scan (SADABS; Bruker, 2007)	$\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 2.6^\circ$
$T_{\text{min}} = 0.899$, $T_{\text{max}} = 0.972$	$h = -8 \rightarrow 8$
7115 measured reflections	$k = -15 \rightarrow 13$
	$l = -18 \rightarrow 16$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.080$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.185$	H-atom parameters constrained
$S = 0.92$	$w = 1/[\sigma^2(F_o^2) + (0.0279P)^2]$
2506 reflections	where $P = (F_o^2 + 2F_c^2)/3$
208 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.2762 (3)	0.18899 (12)	1.41156 (10)	0.0618 (7)
N1	0.2572 (8)	0.4009 (4)	1.4787 (3)	0.0468 (16)
N2	0.5023 (10)	0.0960 (4)	1.7252 (4)	0.065 (2)
O1	0.1367 (7)	0.4326 (3)	1.3208 (3)	0.0730 (18)
H1	0.1721	0.3999	1.3648	0.110*
O2	0.4914 (9)	0.0043 (4)	1.7011 (3)	0.0845 (19)
O3	0.5720 (9)	0.1209 (3)	1.7972 (3)	0.086 (2)
C1	0.2399 (9)	0.5024 (5)	1.4905 (4)	0.0436 (19)
H1A	0.2700	0.5291	1.5456	0.052*
C2	0.1788 (9)	0.5698 (4)	1.4240 (4)	0.0441 (19)
C3	0.1298 (11)	0.5312 (5)	1.3387 (4)	0.058 (2)
C4	0.0772 (10)	0.6039 (5)	1.2683 (4)	0.060 (2)
H4	0.0473	0.5789	1.2127	0.072*
C5	0.0714 (10)	0.7060 (5)	1.2830 (4)	0.060 (2)
H5	0.0401	0.7506	1.2366	0.072*
C6	0.1122 (9)	0.7501 (4)	1.3681 (4)	0.0421 (18)
C7	0.1664 (9)	0.6842 (4)	1.4387 (4)	0.0441 (19)
C8	0.2087 (9)	0.7311 (5)	1.5193 (4)	0.052 (2)
H8	0.2425	0.6894	1.5672	0.062*
C9	0.2017 (10)	0.8362 (5)	1.5295 (5)	0.054 (2)
H9	0.2331	0.8656	1.5836	0.065*
C10	0.1475 (10)	0.8988 (5)	1.4589 (5)	0.056 (2)
H10	0.1407	0.9704	1.4661	0.068*
C11	0.1037 (10)	0.8572 (4)	1.3787 (5)	0.054 (2)
H11	0.0687	0.9002	1.3316	0.065*
C12	0.3140 (9)	0.3279 (4)	1.5437 (4)	0.0400 (18)
C13	0.3278 (9)	0.2238 (5)	1.5197 (4)	0.0413 (18)
C14	0.3845 (10)	0.1468 (4)	1.5788 (4)	0.046 (2)
H14	0.3892	0.0775	1.5624	0.055*
C15	0.4332 (9)	0.1761 (5)	1.6617 (4)	0.0444 (18)
C16	0.4224 (9)	0.2773 (5)	1.6893 (4)	0.047 (2)
H16	0.4532	0.2941	1.7470	0.057*
C17	0.3651 (9)	0.3523 (4)	1.6296 (4)	0.0426 (19)
H17	0.3604	0.4212	1.6470	0.051*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0977 (16)	0.0460 (10)	0.0362 (10)	-0.0018 (11)	-0.0089 (10)	-0.0058 (8)

supplementary materials

N1	0.064 (4)	0.024 (3)	0.048 (4)	0.000 (3)	-0.005 (3)	0.003 (3)
N2	0.103 (6)	0.042 (4)	0.043 (4)	0.001 (4)	-0.013 (4)	0.005 (3)
O1	0.134 (5)	0.037 (3)	0.039 (3)	-0.007 (3)	-0.019 (3)	-0.001 (2)
O2	0.144 (5)	0.043 (3)	0.060 (4)	0.006 (3)	-0.007 (4)	0.004 (3)
O3	0.148 (6)	0.055 (3)	0.040 (3)	0.009 (3)	-0.036 (4)	0.001 (2)
C1	0.051 (5)	0.036 (4)	0.042 (4)	-0.006 (3)	0.002 (4)	0.002 (3)
C2	0.053 (5)	0.037 (4)	0.040 (4)	-0.001 (3)	-0.002 (4)	0.000 (3)
C3	0.084 (6)	0.033 (4)	0.051 (5)	0.007 (4)	-0.008 (5)	-0.003 (3)
C4	0.094 (7)	0.045 (4)	0.032 (4)	0.000 (4)	-0.025 (4)	-0.002 (3)
C5	0.077 (6)	0.048 (5)	0.049 (5)	-0.005 (4)	-0.013 (4)	0.016 (4)
C6	0.050 (5)	0.035 (4)	0.041 (4)	0.005 (3)	0.004 (4)	0.003 (3)
C7	0.051 (5)	0.032 (4)	0.045 (4)	-0.003 (3)	-0.007 (4)	-0.004 (3)
C8	0.062 (5)	0.047 (4)	0.043 (5)	-0.002 (4)	-0.003 (4)	0.008 (3)
C9	0.060 (6)	0.045 (5)	0.053 (5)	0.001 (4)	-0.003 (4)	-0.015 (4)
C10	0.067 (6)	0.030 (4)	0.072 (6)	0.003 (4)	0.008 (5)	-0.010 (4)
C11	0.059 (5)	0.028 (4)	0.070 (6)	0.005 (3)	-0.009 (5)	0.001 (4)
C12	0.046 (5)	0.036 (4)	0.038 (4)	-0.003 (3)	0.006 (4)	-0.003 (3)
C13	0.051 (5)	0.037 (4)	0.034 (4)	-0.003 (3)	0.002 (4)	-0.008 (3)
C14	0.070 (6)	0.029 (4)	0.035 (4)	-0.007 (3)	-0.007 (4)	-0.004 (3)
C15	0.055 (5)	0.042 (4)	0.033 (4)	-0.006 (4)	-0.004 (4)	0.008 (3)
C16	0.062 (5)	0.045 (4)	0.031 (4)	-0.004 (4)	-0.002 (4)	-0.003 (3)
C17	0.053 (5)	0.032 (4)	0.041 (4)	0.001 (3)	-0.001 (4)	-0.008 (3)

Geometric parameters (Å, °)

C11—C13	1.751 (6)	C6—C7	1.408 (8)
N1—C1	1.328 (7)	C7—C8	1.400 (8)
N1—C12	1.406 (7)	C8—C9	1.364 (8)
N2—O3	1.215 (6)	C8—H8	0.9300
N2—O2	1.239 (6)	C9—C10	1.383 (9)
N2—C15	1.471 (7)	C9—H9	0.9300
O1—C3	1.303 (7)	C10—C11	1.368 (9)
O1—H1	0.8200	C10—H10	0.9300
C1—C2	1.383 (8)	C11—H11	0.9300
C1—H1A	0.9300	C12—C17	1.387 (8)
C2—C3	1.429 (8)	C12—C13	1.399 (7)
C2—C7	1.495 (8)	C13—C14	1.380 (7)
C3—C4	1.458 (8)	C14—C15	1.357 (8)
C4—C5	1.335 (8)	C14—H14	0.9300
C4—H4	0.9300	C15—C16	1.379 (8)
C5—C6	1.449 (8)	C16—C17	1.370 (7)
C5—H5	0.9300	C16—H16	0.9300
C6—C11	1.391 (7)	C17—H17	0.9300
C1—N1—C12	125.2 (5)	C7—C8—H8	119.0
O3—N2—O2	122.5 (5)	C8—C9—C10	119.5 (7)
O3—N2—C15	120.1 (6)	C8—C9—H9	120.2
O2—N2—C15	117.3 (6)	C10—C9—H9	120.2
C3—O1—H1	109.5	C11—C10—C9	121.1 (6)
N1—C1—C2	122.4 (6)	C11—C10—H10	119.4

N1—C1—H1A	118.8	C9—C10—H10	119.4
C2—C1—H1A	118.8	C10—C11—C6	119.3 (7)
C1—C2—C3	120.3 (6)	C10—C11—H11	120.3
C1—C2—C7	121.2 (6)	C6—C11—H11	120.3
C3—C2—C7	118.5 (5)	C17—C12—C13	117.5 (5)
O1—C3—C2	122.1 (6)	C17—C12—N1	124.7 (5)
O1—C3—C4	118.3 (6)	C13—C12—N1	117.8 (6)
C2—C3—C4	119.6 (6)	C14—C13—C12	122.0 (6)
C5—C4—C3	120.7 (6)	C14—C13—C11	118.2 (5)
C5—C4—H4	119.6	C12—C13—C11	119.7 (5)
C3—C4—H4	119.6	C15—C14—C13	117.3 (6)
C4—C5—C6	122.6 (6)	C15—C14—H14	121.3
C4—C5—H5	118.7	C13—C14—H14	121.3
C6—C5—H5	118.7	C14—C15—C16	123.3 (6)
C11—C6—C7	120.9 (6)	C14—C15—N2	118.3 (6)
C11—C6—C5	119.5 (6)	C16—C15—N2	118.3 (6)
C7—C6—C5	119.5 (5)	C17—C16—C15	118.2 (6)
C8—C7—C6	117.2 (6)	C17—C16—H16	120.9
C8—C7—C2	123.8 (6)	C15—C16—H16	120.9
C6—C7—C2	119.0 (5)	C16—C17—C12	121.5 (6)
C9—C8—C7	121.9 (6)	C16—C17—H17	119.2
C9—C8—H8	119.0	C12—C17—H17	119.2
C12—N1—C1—C2	-178.4 (7)	C8—C9—C10—C11	-1.1 (11)
N1—C1—C2—C3	0.6 (11)	C9—C10—C11—C6	0.6 (12)
N1—C1—C2—C7	-178.1 (6)	C7—C6—C11—C10	-0.5 (11)
C1—C2—C3—O1	1.4 (12)	C5—C6—C11—C10	-178.2 (7)
C7—C2—C3—O1	-179.9 (6)	C1—N1—C12—C17	-1.8 (11)
C1—C2—C3—C4	-176.2 (7)	C1—N1—C12—C13	-179.0 (6)
C7—C2—C3—C4	2.5 (11)	C17—C12—C13—C14	1.9 (10)
O1—C3—C4—C5	-178.7 (7)	N1—C12—C13—C14	179.2 (6)
C2—C3—C4—C5	-1.0 (11)	C17—C12—C13—C11	-177.0 (5)
C3—C4—C5—C6	-1.4 (11)	N1—C12—C13—C11	0.4 (8)
C4—C5—C6—C11	179.9 (7)	C12—C13—C14—C15	-2.1 (11)
C4—C5—C6—C7	2.2 (11)	C11—C13—C14—C15	176.7 (5)
C11—C6—C7—C8	0.8 (10)	C13—C14—C15—C16	2.2 (11)
C5—C6—C7—C8	178.5 (6)	C13—C14—C15—N2	-177.3 (6)
C11—C6—C7—C2	-178.3 (6)	O3—N2—C15—C14	169.8 (7)
C5—C6—C7—C2	-0.6 (10)	O2—N2—C15—C14	-8.1 (10)
C1—C2—C7—C8	-2.0 (10)	O3—N2—C15—C16	-9.8 (11)
C3—C2—C7—C8	179.3 (7)	O2—N2—C15—C16	172.3 (7)
C1—C2—C7—C6	177.0 (7)	C14—C15—C16—C17	-2.0 (11)
C3—C2—C7—C6	-1.7 (10)	N2—C15—C16—C17	177.5 (6)
C6—C7—C8—C9	-1.2 (11)	C15—C16—C17—C12	1.7 (10)
C2—C7—C8—C9	177.7 (6)	C13—C12—C17—C16	-1.6 (10)
C7—C8—C9—C10	1.4 (11)	N1—C12—C17—C16	-178.8 (6)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
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supplementary materials

O1—H1···N1	0.82	1.81	2.547 (5)	149
C8—H8···O3 ⁱ	0.93	2.50	3.392 (5)	160

Symmetry codes: (i) $-x+1, y+1/2, -z+7/2$.

Fig. 1

