

**(E)-2-[2-(Hydroxymethyl)phenylimino-methyl]-6-methylphenol**Zarife Sibel Gül,<sup>a\*</sup> Ferda Erşahin,<sup>b</sup> Erbil Açar<sup>b</sup> and Şamil Işık<sup>a</sup><sup>a</sup>Department of Physics, Ondokuz Mayıs University, TR-55139 Samsun, Turkey, and<sup>b</sup>Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

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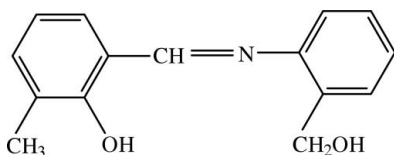
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Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.041;  $wR$  factor = 0.085; data-to-parameter ratio = 8.9.

The molecule of the title compound,  $\text{C}_{15}\text{H}_{15}\text{NO}_2$ , is not planar, displaying a dihedral angle of  $21.21(18)^\circ$  between the two aromatic rings. The central  $\text{N}=\text{C}$  bond distance of  $1.279(4)$  Å is typical for an imine double bond. There are intramolecular  $\text{O}-\text{H}\cdots\text{N}$  and intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds.

**Related literature**

Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Hadjoudis *et al.*, 1987). Structures related to the title compound may be found in: Ersanlı *et al.* (2004); Gül *et al.* (2007). For applications of related Schiff bases, see: Sabater *et al.* (2001); Di Bella (2001).

**Experimental***Crystal data* $\text{C}_{15}\text{H}_{15}\text{NO}_2$  $M_r = 241.28$ Orthorhombic,  $P2_12_12_1$  $a = 4.7829(4)$  Å $b = 12.7379(13)$  Å $c = 20.532(2)$  Å $V = 1250.9(2)$  Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.09$  mm<sup>-1</sup> $T = 296$  K $0.80 \times 0.70 \times 0.46$  mm*Data collection*

Stoe IPDS II diffractometer

Absorption correction: integration

 $(X\text{-RED32; Stoe \& Cie, 2002})$  $T_{\min} = 0.958, T_{\max} = 0.994$ 

11194 measured reflections

1460 independent reflections

787 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.129$ *Refinement* $R[F^2 > 2\sigma(F^2)] = 0.041$  $wR(F^2) = 0.085$  $S = 0.79$ 

1460 reflections

164 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.13$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.15$  e Å<sup>-3</sup>**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	1.86	2.595 (4)	148
$\text{O2}-\text{H2A}\cdots\text{O2}^i$	0.82	1.93	2.6983 (18)	155

Symmetry code: (i)  $x + \frac{1}{2}, -y + \frac{5}{2}, -z$ .

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).

The authors are grateful to the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for use of the Stoe IPDS II diffractometer (purchased under grant No. F279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2113).

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**supplementary materials**

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## (*E*)-2-[2-(Hydroxymethyl)phenyliminomethyl]-6-methylphenol

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### Comment

In this paper we present the crystal and molecular structures of a Schiff base, C<sub>15</sub>H<sub>15</sub>NO<sub>2</sub>. Recently, Schiff bases have been widely investigated for their properties and applications in different fields, such as catalysis and materials chemistry (Sabater *et al.*, 2001; Di Bella, 2001). Schiff bases derived from 2-hydroxy-1-naphthaldehyde with various alkyl or aryl *N*-substituents, apart from excellent donor abilities, exhibit interesting photo- and thermo-chromic features. There are two types of intramolecular hydrogen bonds in Schiff bases, which may be stabilized in keto–amine (N—H···O hydrogen bond) or phenol–imine (N···H—O hydrogen bond) tautomeric forms. The present X-ray investigation shows that the title compound exists in the phenol–imine form (Fig. 1).

The C1—N1 and C7—C8 bond lengths are 1.408 (4) and 1.442 (4) Å, respectively, and agree with the corresponding distances in (*E*)-2-[4-(dimethylamino)phenyliminomethyl]-6-methylphenol [1.412 (2) and 1.441 (3) Å; Gül *et al.*, 2007]. The C7=N1 and O1—C13 bond lengths are 1.279 (4) and 1.357 (4) Å, respectively, and agree with the corresponding distances in 2-[2-(hydroxymethyl)phenyliminomethyl]phenol [1.275 (2) and 1.354 (2) Å; Ersanlı *et al.*, 2004]. Fig.1 also shows a strong intramolecular hydrogen bond, O1—H1···N1, describing a *S*(6) motif. Atom O2 in the asymmetric unit acts as hydrogen-bond donor, *via* H2A, connecting this molecule to O2 in a symmetry related molecule at ( $x + 1/2, -y + 5/2, -z$ ), forming a *C*(2) chain running parallel to the [100] direction (Fig. 2).

### Experimental

The title compound was prepared by refluxing a mixture of a solution containing 3-methylsalicylaldehyde (0.1 ml, 0.82 mmol) in 20 ml ethanol and a solution containing 2-aminobenzylalcohol (0.1 g, 0.82 mmol) in 20 ml ethanol. The reaction mixture was refluxed for 1 h. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethylalcohol solution (yield 15%; m.p. 377–379 K).

### Refinement

H atoms of the hydroxyl groups were refined with O—H constrained to 0.82 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H = 0.93–0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  or  $1.5U_{\text{eq}}(\text{C})$ . 986 measured Friedel pairs were merged before the final refinement cycles.

### Figures



Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

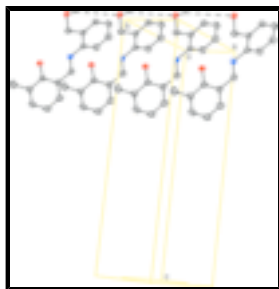


Fig. 2. A packing diagram of the title compound; dashed lines indicate hydrogen bonds. Other H atoms are omitted for clarity.

## (E)-2-[2-(Hydroxymethyl)phenyliminomethyl]-6-methylphenol

### Crystal data

$C_{15}H_{15}NO_2$

$M_r = 241.28$

Orthorhombic,  $P2_12_12_1$

Hall symbol: P 2ac 2ab

$a = 4.7829$  (4) Å

$b = 12.7379$  (13) Å

$c = 20.532$  (2) Å

$V = 1250.9$  (2) Å<sup>3</sup>

$Z = 4$

$F_{000} = 512$

$D_x = 1.281$  Mg m<sup>-3</sup>

Melting point: 377–379 K

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 8449 reflections

$\theta = 1.9$ – $29.1^\circ$

$\mu = 0.09$  mm<sup>-1</sup>

$T = 296$  K

Prism, yellow

$0.80 \times 0.70 \times 0.46$  mm

### Data collection

Stoe IPDSII  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 6.67 pixels mm<sup>-1</sup>

$T = 296$  K

$\omega$  scans

Absorption correction: integration  
(X-RED32; Stoe & Cie, 2002)

$T_{\min} = 0.958$ ,  $T_{\max} = 0.994$

11194 measured reflections

1460 independent reflections

787 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.129$

$\theta_{\max} = 26.0^\circ$

$\theta_{\min} = 1.9^\circ$

$h = -5 \rightarrow 5$

$k = -15 \rightarrow 15$

$l = -25 \rightarrow 25$

### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.041$

$wR(F^2) = 0.085$

H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.13$  e Å<sup>-3</sup>

$S = 0.79$

$\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$

1460 reflections

Extinction correction: none

164 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.0147 (6)	0.98344 (19)	0.15542 (13)	0.0447 (7)
O1	-0.3647 (5)	1.11069 (18)	0.19932 (10)	0.0582 (8)
H1	-0.2500	1.0866	0.1737	0.087*
O2	0.1874 (5)	1.20510 (16)	0.01226 (10)	0.0573 (7)
H2A	0.3534	1.2131	0.0036	0.086*
C7	0.0035 (8)	0.9353 (3)	0.21002 (16)	0.0485 (9)
H7	0.1295	0.8811	0.2179	0.058*
C15	0.1614 (8)	1.1426 (2)	0.06926 (15)	0.0547 (11)
H15A	-0.0352	1.1359	0.0801	0.066*
H15B	0.2531	1.1782	0.1051	0.066*
C9	-0.2145 (9)	0.9028 (3)	0.31711 (16)	0.0616 (11)
H9	-0.0983	0.8450	0.3227	0.074*
C8	-0.1973 (7)	0.9619 (3)	0.25972 (15)	0.0436 (8)
C12	-0.5574 (8)	1.0792 (3)	0.30303 (17)	0.0509 (10)
C11	-0.5665 (9)	1.0168 (3)	0.35773 (18)	0.0632 (12)
H11	-0.6897	1.0344	0.3910	0.076*
C6	0.2859 (7)	1.0336 (2)	0.06216 (15)	0.0413 (8)
C1	0.2078 (7)	0.9556 (2)	0.10665 (15)	0.0431 (8)
C13	-0.3729 (7)	1.0500 (3)	0.25363 (16)	0.0448 (9)
C5	0.4738 (8)	1.0091 (3)	0.01373 (16)	0.0519 (9)
H5	0.5264	1.0610	-0.0157	0.062*
C4	0.5866 (8)	0.9100 (3)	0.00754 (18)	0.0568 (10)
H4	0.7146	0.8955	-0.0253	0.068*
C2	0.3168 (8)	0.8544 (3)	0.09890 (18)	0.0565 (10)
H2	0.2597	0.8010	0.1268	0.068*
C10	-0.3997 (9)	0.9290 (3)	0.36505 (17)	0.0668 (12)
H10	-0.4134	0.8880	0.4024	0.080*
C14	-0.7375 (9)	1.1733 (3)	0.29493 (19)	0.0725 (12)
H14A	-0.8577	1.1803	0.3321	0.109*
H14B	-0.8489	1.1658	0.2563	0.109*
H14C	-0.6222	1.2347	0.2911	0.109*
C3	0.5070 (9)	0.8330 (3)	0.05063 (17)	0.0609 (10)
H3	0.5825	0.7660	0.0470	0.073*

## supplementary materials

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### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0486 (17)	0.0428 (17)	0.0428 (15)	-0.0050 (15)	0.0044 (16)	0.0048 (14)
O1	0.0690 (19)	0.0568 (15)	0.0487 (14)	0.0052 (13)	0.0006 (13)	0.0111 (12)
O2	0.0561 (16)	0.0578 (14)	0.0579 (14)	0.0031 (13)	0.0006 (15)	0.0247 (13)
C7	0.047 (2)	0.040 (2)	0.059 (2)	-0.0056 (19)	-0.002 (2)	0.0025 (17)
C15	0.067 (3)	0.051 (2)	0.046 (2)	0.005 (2)	0.002 (2)	0.0148 (17)
C9	0.082 (3)	0.051 (2)	0.052 (2)	-0.009 (2)	-0.005 (2)	0.011 (2)
C8	0.046 (2)	0.044 (2)	0.0408 (19)	-0.0072 (19)	-0.0001 (18)	0.0064 (17)
C12	0.049 (3)	0.056 (2)	0.048 (2)	-0.007 (2)	-0.002 (2)	-0.0088 (19)
C11	0.062 (3)	0.080 (3)	0.048 (2)	-0.011 (3)	0.008 (2)	-0.009 (2)
C6	0.041 (2)	0.044 (2)	0.0385 (18)	-0.0017 (18)	-0.0012 (17)	0.0007 (16)
C1	0.043 (2)	0.042 (2)	0.0440 (19)	-0.0018 (19)	-0.0028 (18)	0.0028 (16)
C13	0.045 (2)	0.050 (2)	0.0393 (18)	-0.0083 (19)	-0.0022 (18)	0.0036 (18)
C5	0.057 (2)	0.054 (2)	0.044 (2)	-0.003 (2)	0.004 (2)	0.0060 (17)
C4	0.059 (3)	0.057 (2)	0.055 (2)	0.002 (2)	0.010 (2)	-0.009 (2)
C2	0.065 (3)	0.041 (2)	0.064 (2)	-0.002 (2)	0.006 (2)	0.0025 (18)
C10	0.080 (3)	0.077 (3)	0.043 (2)	-0.020 (3)	0.004 (2)	0.014 (2)
C14	0.066 (3)	0.068 (3)	0.083 (3)	0.008 (2)	0.001 (3)	-0.016 (2)
C3	0.067 (3)	0.046 (2)	0.069 (2)	0.000 (2)	0.005 (3)	-0.007 (2)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

N1—C7	1.279 (4)	C12—C14	1.485 (5)
N1—C1	1.408 (4)	C11—C10	1.382 (5)
O1—C13	1.357 (4)	C11—H11	0.9300
O1—H1	0.8200	C6—C5	1.376 (4)
O2—C15	1.421 (3)	C6—C1	1.400 (4)
O2—H2A	0.8200	C1—C2	1.399 (5)
C7—C8	1.442 (4)	C5—C4	1.378 (5)
C7—H7	0.9300	C5—H5	0.9300
C15—C6	1.517 (4)	C4—C3	1.375 (5)
C15—H15A	0.9700	C4—H4	0.9300
C15—H15B	0.9700	C2—C3	1.373 (5)
C9—C10	1.365 (5)	C2—H2	0.9300
C9—C8	1.400 (4)	C10—H10	0.9300
C9—H9	0.9300	C14—H14A	0.9600
C8—C13	1.408 (4)	C14—H14B	0.9600
C12—C11	1.377 (5)	C14—H14C	0.9600
C12—C13	1.395 (4)	C3—H3	0.9300
C7—N1—C1	122.0 (3)	C2—C1—C6	118.7 (3)
C13—O1—H1	109.5	C2—C1—N1	123.9 (3)
C15—O2—H2A	109.5	C6—C1—N1	117.4 (3)
N1—C7—C8	122.4 (3)	O1—C13—C12	117.6 (3)
N1—C7—H7	118.8	O1—C13—C8	120.7 (3)
C8—C7—H7	118.8	C12—C13—C8	121.7 (3)

O2—C15—C6	113.5 (3)	C6—C5—C4	122.0 (3)
O2—C15—H15A	108.9	C6—C5—H5	119.0
C6—C15—H15A	108.9	C4—C5—H5	119.0
O2—C15—H15B	108.9	C3—C4—C5	119.1 (4)
C6—C15—H15B	108.9	C3—C4—H4	120.5
H15A—C15—H15B	107.7	C5—C4—H4	120.5
C10—C9—C8	120.9 (4)	C3—C2—C1	120.8 (3)
C10—C9—H9	119.5	C3—C2—H2	119.6
C8—C9—H9	119.5	C1—C2—H2	119.6
C9—C8—C13	117.9 (3)	C9—C10—C11	119.6 (4)
C9—C8—C7	120.6 (3)	C9—C10—H10	120.2
C13—C8—C7	121.5 (3)	C11—C10—H10	120.2
C11—C12—C13	117.3 (4)	C12—C14—H14A	109.5
C11—C12—C14	122.6 (4)	C12—C14—H14B	109.5
C13—C12—C14	120.0 (3)	H14A—C14—H14B	109.5
C12—C11—C10	122.5 (4)	C12—C14—H14C	109.5
C12—C11—H11	118.7	H14A—C14—H14C	109.5
C10—C11—H11	118.7	H14B—C14—H14C	109.5
C5—C6—C1	119.0 (3)	C2—C3—C4	120.4 (4)
C5—C6—C15	122.2 (3)	C2—C3—H3	119.8
C1—C6—C15	118.8 (3)	C4—C3—H3	119.8
C1—N1—C7—C8	-178.7 (3)	C14—C12—C13—O1	0.4 (5)
C10—C9—C8—C13	1.2 (5)	C11—C12—C13—C8	-1.5 (5)
C10—C9—C8—C7	178.5 (3)	C14—C12—C13—C8	179.5 (3)
N1—C7—C8—C9	175.9 (3)	C9—C8—C13—O1	179.6 (3)
N1—C7—C8—C13	-7.0 (5)	C7—C8—C13—O1	2.3 (4)
C13—C12—C11—C10	0.7 (6)	C9—C8—C13—C12	0.6 (5)
C14—C12—C11—C10	179.7 (4)	C7—C8—C13—C12	-176.7 (3)
O2—C15—C6—C5	17.9 (5)	C1—C6—C5—C4	0.3 (5)
O2—C15—C6—C1	-162.4 (3)	C15—C6—C5—C4	179.9 (3)
C5—C6—C1—C2	-2.1 (5)	C6—C5—C4—C3	0.6 (6)
C15—C6—C1—C2	178.2 (3)	C6—C1—C2—C3	3.1 (5)
C5—C6—C1—N1	-179.9 (3)	N1—C1—C2—C3	-179.3 (3)
C15—C6—C1—N1	0.5 (4)	C8—C9—C10—C11	-2.0 (6)
C7—N1—C1—C2	27.9 (5)	C12—C11—C10—C9	1.0 (6)
C7—N1—C1—C6	-154.5 (3)	C1—C2—C3—C4	-2.2 (6)
C11—C12—C13—O1	179.4 (3)	C5—C4—C3—C2	0.3 (6)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 $\cdots$ N1	0.82	1.86	2.595 (4)	148
O2—H2A $\cdots$ O2 <sup>i</sup>	0.82	1.93	2.6983 (18)	155

Symmetry codes: (i)  $x+1/2, -y+5/2, -z$ .

Fig. 1

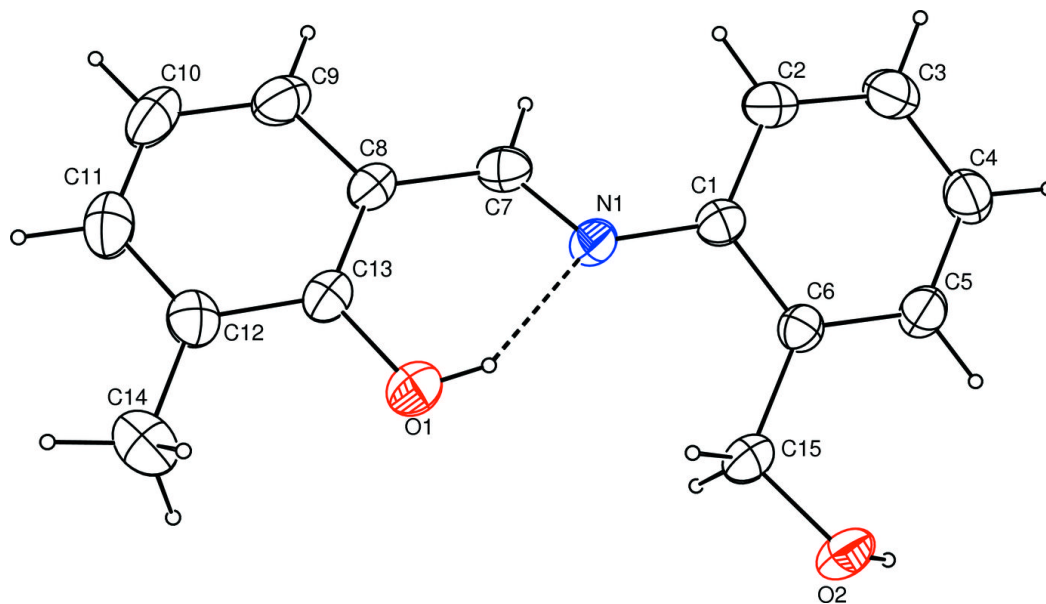


Fig. 2

