Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*E*)-2-[2-(Hydroxymethyl)phenylimino-methyl]-6-methylphenol

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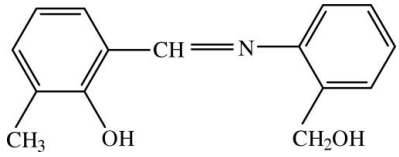
Received 30 May 2007; accepted 2 July 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.041; wR factor = 0.085; data-to-parameter ratio = 8.9.

The molecule of the title compound, $C_{15}H_{15}NO_2$, is not planar, displaying a dihedral angle of 21.21 (18)° between the two aromatic rings. The central N=C bond distance of 1.279 (4) Å is typical for an imine double bond. There are intramolecular O—H···N and intermolecular O—H···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

$C_{15}H_{15}NO_2$
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^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.80 × 0.70 × 0.46 mm

Data collection

Stoe IPDS II diffractometer
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_{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
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.86	2.595 (4)	148
O2—H2A···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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 doi:10.1107/S1600536807032266

supplementary materials

Acta Cryst. (2007). E**63**, o3547 [**doi:10.1107/S1600536807032266**]

(*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, $C_{15}H_{15}NO_2$. 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 e thanol and a solution containing 2-aminobenzylalcohol (0.1 g, 0.82 mmol) in 20 ml e thanol. 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_{iso}(H) = 1.5U_{eq}(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_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). 986 measured Friedel pairs were merged before the final refinement cycles.

Figures

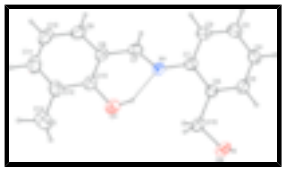

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level.

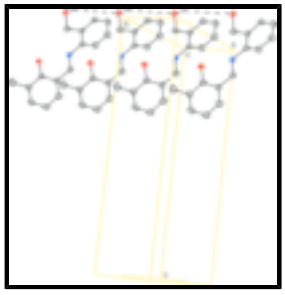

Fig. 2. A packing diagram of the title compound; dashed lines indicate hydrogen bonds. Other H atoms are omitted for clarity.

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

Crystal data

$C_{15}H_{15}NO_2$	$D_x = 1.281$ Mg m^{-3}
$M_r = 241.28$	Melting point: 377–379 K
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 8449 reflections
$a = 4.7829$ (4) Å	$\theta = 1.9$–29.1^o
$b = 12.7379$ (13) Å	$\mu = 0.09$ mm^{-1}
$c = 20.532$ (2) Å	$T = 296$ K
$V = 1250.9$ (2) Å^3	Prism, yellow
$Z = 4$	0.80 × 0.70 × 0.46 mm
$F_{000} = 512$	

Data collection

Stoe IPDSII diffractometer	1460 independent reflections
Radiation source: fine-focus sealed tube	787 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.129$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 26.0^o$
$T = 296$ K	$\theta_{min} = 1.9^o$
ω scans	$h = -5 \rightarrow 5$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$k = -15 \rightarrow 15$
$T_{min} = 0.958$, $T_{max} = 0.994$	$l = -25 \rightarrow 25$
11194 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.041$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.085$	$\Delta\rho_{max} = 0.13$ e Å^{-3}

$S = 0.79$

1460 reflections

164 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$\Delta\rho_{min} = -0.15$ e Å^{-3}

Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{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*

Atomic displacement parameters (Å^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 (Å, °)

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 (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.86	2.595 (4)	148
O2—H2A···O2^{i}	0.82	1.93	2.6983 (18)	155

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

Fig. 1

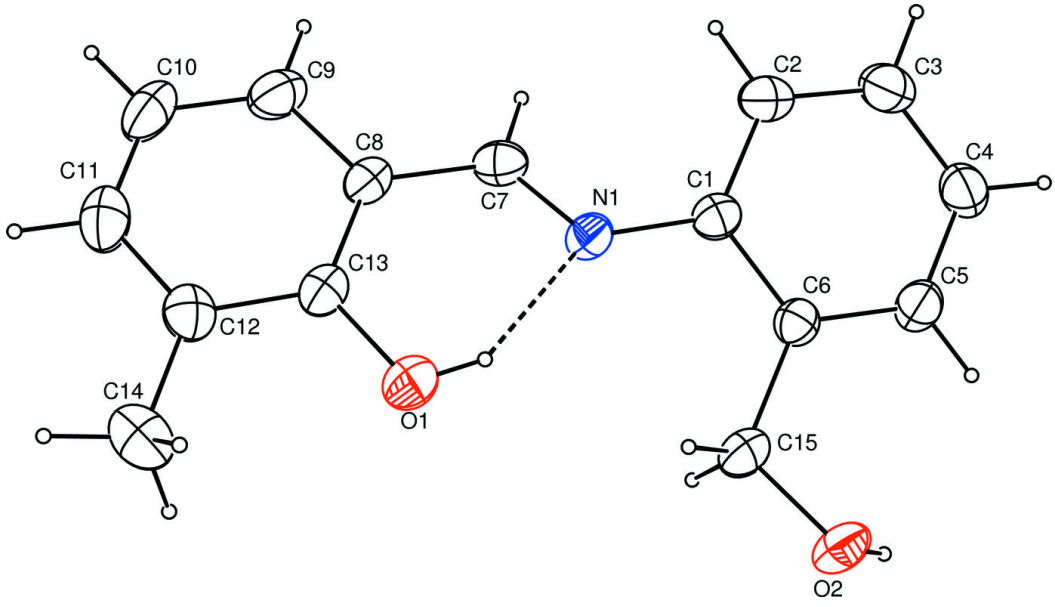

Fig. 2