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2-[2-(Hydroxymethyl)phenyliminomethyl]-phenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.044
wR factor = 0.108
Data-to-parameter ratio = 15.2

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

Molecules of the title compound, $C_{14}H_{13}NO_2$, are nearly planar. The molecular structure is stabilized by a strong intramolecular O—H···N hydrogen bond between the imine and hydroxyl groups [O···N = 2.614 (2) Å]. In the crystal structure, intermolecular O—H···O hydrogen bonds [O···O = 2.681 (3) and 2.641 (3) Å] link inversion-related molecules into chains parallel to the *a* axis.

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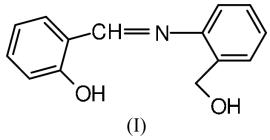
Comment

Although many structures of transition metal complexes with Schiff bases have been determined, a relatively small number of free Schiff bases have been structurally characterized (Calligaris & Randaccio, 1987). *N*-Substituted salicylaldimines are also of interest because of their thermochromism and photochromism in the solid state, which may involve reversible proton transfer from the hydroxyl O atom to the imine N atom (Moustakali *et al.*, 1978; Hadjoudis *et al.*, 1987; Xu *et al.*, 1994) and charge transport occurs through intermolecular overlap between π orbitals with proton transfer; the proton transfer may also be a basis for the development of molecular switches (Xu *et al.*, 1994). On the basis of some thermochromic and photochromic Schiff base compounds, it was proposed that molecules exhibiting thermochromism are planar, while those exhibiting photochromism are non-planar (Moustakali *et al.*, 1978), and that planarity of the molecule facilitates proton transfer through the hydrogen bond in the ground state with a small energy requirement (Bregman *et al.*, 1964).



(I)

In the course of a systematic structural investigation of Schiff bases (Kazak *et al.*, 2000; Ersanlı *et al.*, 2003; Odabaşoğlu, Albayrak, Büyükgüngör & Goesmann, 2003) the

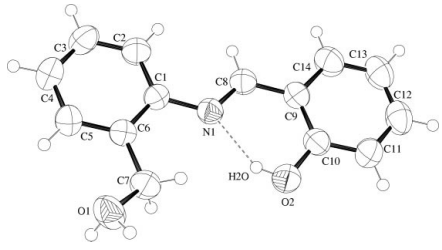


Figure 1
A view of the molecule of (I), showing the atom-labelling scheme, with displacement ellipsoids drawn at the 50% probability level. The H atom attached to O1 is disordered over two positions, each with occupancy of 0.5; both are shown.

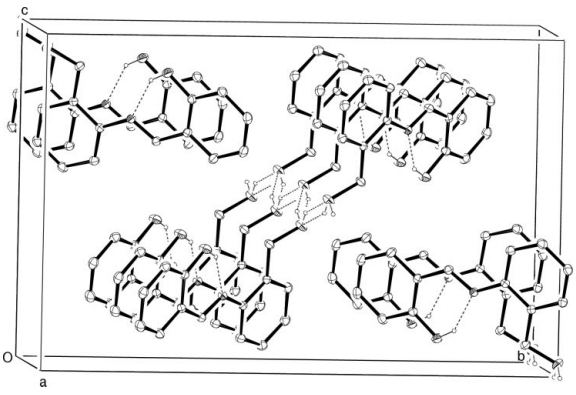


Figure 2
A packing diagram of (I), showing the hydrogen-bonding scheme and disorder in one H atom. Short H···H contacts result if there is no disorder. With the exception of atoms H1*A*, H1*B* and H2O, H atoms have been omitted for clarity.

structure of the title compound, (I), was determined. An *ORTEP*-3 (Farrugia, 1997) view of the molecule of (I) and a packing diagram are shown in Figs. 1 and 2, respectively.

Two types of intramolecular hydrogen bonds (N—H···O or O—H···N) can exist in Schiff bases (Garnovskii *et al.*, 1993). Clearly, the enol–imine tautomer is favoured over the keto–imine form. This is evident from the observed O2—C10 bond distance of 1.354 (2) Å, which is consistent with an O—C single bond; similarly, the N1—C8 distance of 1.275 (2) Å is consistent with an N═C double bond, as in 2-salicylideneamino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carbonitrile [C—O = 1.360 (2) Å and N═C = 1.281 (2) Å; Elerman & Elmalı, 1998] and 2-[(4-hydroxyphenyl)iminomethyl]thiophene [C—O = 1.358 (2) Å and N═C = 1.282 (2) Å; Kazak *et al.*, 2000]. A strong O—H···N intramolecular hydrogen bond [O2···N1 = 2.614 (2) Å] is observed in the molecular structure. The sum of the van der Waals radii of O and N (3.07 Å; Bondi, 1964) atoms is significantly longer than the O···N distance, which is similar to the O···N distances in thermochromic 2,2′-azinodimethyldiphenol [2.611 (6) Å; Xu *et al.*, 1994], bis-*N,N′*-*p*-chlorosalicylideneamine-1,2-diaminobenzene [2.615 (6) Å; Elerman *et al.*, 1994] and *N,N′*-disalicylidene-1,6-pyrenediamine [2.614 (5) Å; Inabe *et al.*, 1989].

The dihedral angle $\theta1$, between the mean planes of the benzene ring (C1–C6) and the C1—N1═C8—C9 group is 2.98 (14)°, and the angle, $\theta2$, between the C1—N1═C8—C9 group and the benzene ring (C9–C14) is 1.67 (13)°. The angle, $\theta3$, between the planes of the rings is 4.63 (10)°, *i.e.* the benzene rings are approximately coplanar.

In the crystal structure, inversion-related molecules are linked by O—H···O hydrogen bonds (Table 2), involving the disordered atoms H1*A* and H1*B*, forming molecular chains along the *a* axis (Fig. 2).

Experimental

The title compound was obtained as described in our previous work (Odabaşoğlu, Albayrak, Büyükgüngör & Lönnecke, 2003). For the X-ray diffraction analysis, suitable single crystals of compound (I) were obtained after 2 d by slow evaporation from an ethyl alcohol solution (yield 85%; m.p. 392–393 K).

Crystal data

$C_{14}H_{13}NO_2$
M_r = 227.25
Monoclinic, $P2_1/n$
a = 4.5866 (4) Å
b = 19.742 (2) Å
c = 12.6200 (11) Å
β = 94.872 (7)°
V = 1138.60 (18) Å^3
Z = 4
D_x = 1.326 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5263 reflections
θ = 1.6–26.8°
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, yellow
0.33 × 0.22 × 0.13 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)
T_{min} = 0.974, T_{max} = 0.988
11355 measured reflections
2471 independent reflections
1329 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 27.1°
$h = -5 \rightarrow 5$
$k = -25 \rightarrow 25$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.108
S = 0.89
2471 reflections
163 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.420 (2)	N1—C8	1.275 (2)
O2—C10	1.354 (2)	N1—C1	1.421 (2)
C8—N1—C1	122.2 (2)	N1—C8—C9	122.2 (2)
C2—C1—N1	124.5 (2)	O2—C10—C11	118.5 (2)
C6—C1—N1	116.1 (2)	O2—C10—C9	121.3 (2)
O1—C7—C6	112.7 (2)		
C8—N1—C1—C2	2.2 (2)	C1—N1—C8—C9	177.60 (14)
N1—C1—C6—C7	−1.1 (2)	N1—C8—C9—C10	1.4 (2)
C5—C6—C7—O1	−18.2 (2)	C8—C9—C10—O2	0.5 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···O1^{i}	0.82 (1)	1.90 (3)	2.681 (3)	158 (7)
O1—H1*B*···O1^{ii}	0.82 (1)	1.87 (3)	2.641 (3)	155 (6)
O2—H2O···N1	0.82	1.89	2.614 (2)	147
C5—H5···O1	0.93	2.48	2.804 (3)	101

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $1-x, 1-y, 1-z$.

All H atoms were placed in calculated positions (O—H = 0.82 Å and C—H = 0.93–0.97 Å), with U_{iso} values constrained to be $1.5U_{eq}$ of the carrier atom for the hydroxyl-group H atom and $1.2U_{eq}$ for the remaining H atoms, expect for the H atom attached to atom O1. This H atom shows positional disorder over two sites, H1*A* and H1*B*, with occupation factors of 0.5. Actually, it is disordered across an inversion centre, *i.e.* H1*A* is attached to one of the two inversion-related O1 atoms and H1*B* to the other. Three reflections showing very bad agreement between F_o and F_c, *viz.* (002), ($\bar{1}$32) and ($\bar{1}$41), were omitted during the final cycles of refinement.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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