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2-[(*E*)-2-(4-Hydroxyphenyl)ethylimino-methyl]phenol

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Key indicators

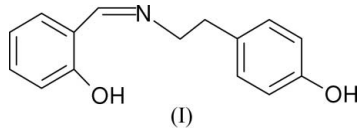
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.061
wR factor = 0.197
Data-to-parameter ratio = 15.4

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

The title compound, $C_{15}H_{15}NO_2$, has been synthesized and characterized by elemental analysis and single-crystal X-ray diffraction. In the crystal structure, the molecules are linked *via* intermolecular O—H···O hydrogen bonds into a zigzag chain structure along the *b* axis.

Comment

Lewis base adducts of the salicylidene group that are derived from the condensation of salicylaldehyde and various primary amines are very interesting in a large number of transition metal complexes (Henson *et al.*, 1999; Zhu, Lin *et al.*, 2003; Zhu, Zeng *et al.*, 2003). Recently, we have reported a Schiff base compound derived from the condensation of salicylaldehyde with *o*-toluidine, which has been structurally characterized (Cheng *et al.*, 2005). As an extension of our work, the crystal structure of the title compound, (I), is reported here.



(I)

In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The torsion angle C7—N1—C8—C9 is 122.6 (2)°. The C7═N1 bond length of 1.283 (3) Å is greater than the value of 1.274 (2) Å observed in the previously cited compound, as a result of the presence of a stronger intramolecular O—H···N interaction (Table 1).

In the crystal structure, the molecules are linked *via* intermolecular O—H···O hydrogen bonds (Table 1) into a zigzag chain structure along the *b* axis, forming layers parallel to the *ac* plane (Fig. 2).

Experimental

p-Tyramine and salicylaldehyde were available commercially and were used without further purification. *p*-Tyramine (1 mmol, 137 mg)

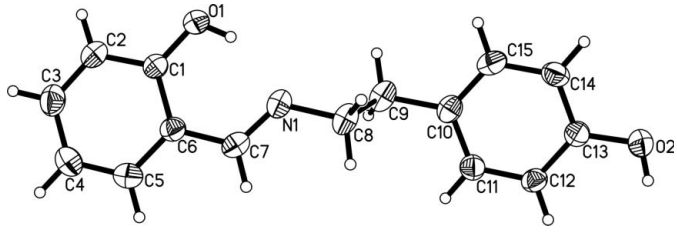


Figure 1
The structure of the title compound (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

and salicylaldehyde (1 mmol, 122 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for 2 h to give a clear brown solution. After allowing the solution to stand in air for 8 d, brown block-shaped crystals were formed, in about 43% yield, on slow evaporation of the solvent. Analysis calculated for $C_{15}H_{15}NO_2$: C 74.67, H 6.27, N 5.81%; found: C 74.66, H 6.29, N 5.80%.

Crystal data

$C_{15}H_{15}NO_2$	D_x = 1.241 Mg m^{-3}
M_r = 241.28	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3701 reflections
a = 15.9378 (13) Å	θ = 3.0–25.2°
b = 12.9460 (10) Å	μ = 0.08 mm^{-1}
c = 14.5886 (12) Å	T = 292 (2) K
β = 120.8650 (10)°	Block, brown
V = 2583.8 (4) Å^3	0.30 × 0.20 × 0.20 mm
Z = 8	

Data collection

Bruker APEX area-detector diffractometer	1931 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.046
Absorption correction: none	θ_{max} = 26.0°
13287 measured reflections	$h = -19 \rightarrow 19$
2545 independent reflections	$k = -15 \rightarrow 15$
	$l = -17 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.1177P)^2 + 0.463P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.061	
$wR(F^2)$ = 0.197	
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
2545 reflections	$\Delta\rho_{max}$ = 0.57 e Å^{-3}
165 parameters	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.82	2.558 (2)	150
O2—H2A···O1^{i}	0.82	1.91	2.725 (2)	173

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

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and O—H distances of 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

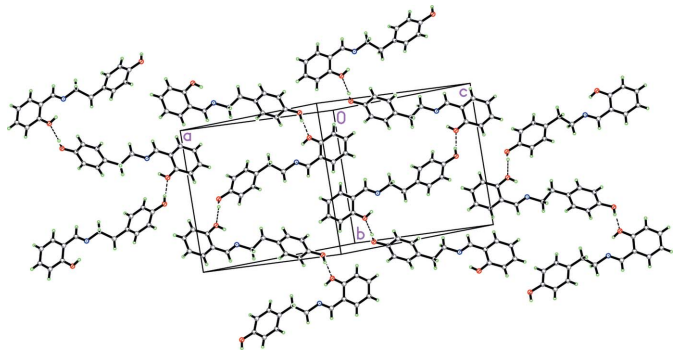


Figure 2
The zigzag chains formed by the molecules of (I), linked *via* intermolecular O—H···O hydrogen bonds (dashed lines).

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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