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2-{(*Z*)-2-[(*E*)-1-(2-Hydroxyphenyl)methylidene]hydrazono}-1,2-diphenylethan-1-one

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Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.125
Data-to-parameter ratio = 14.3

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

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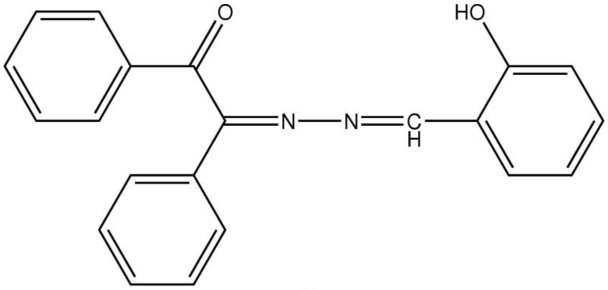
The title compound, $C_{21}H_{15}N_2O_2$, contains two benzene rings (the phenolic ring and the nearest benzene ring) connected through an azine group that show a little deviation from coplanarity. There is an intramolecular hydrogen bond involving the phenol hydroxyl group and the nearest N atom in the azine chain [O—H$\cdots$N = 2.608 (2) Å].

Comment

Schiff base compounds were reported for the first time by Hugo Schiff in 1864 (Carey, 2003). They easily form stable complexes with most transition metal ions, which are of much interest in bioinorganic chemistry due to their pharmacological activities (Refat *et al.*, 2006). In the present paper, we report the synthesis and crystal structure of a new derivative of salicylaldimine Schiff base ligands. Salicylaldimines are of interest due to their important role in biological systems (Yamada, 1999).



(I)

The molecular structure of (I) and the atom-numbering scheme are shown in Fig. 1. A relatively strong intramolecular hydrogen bond is present between the phenol hydroxy group (O1) and the nearest N atom (N2) in the azine chain, leading to a nearly planar hydrogen-bonded ring. The O$\cdots$N contact distances in the title compound [O1—H1$\cdots$N2 = 2.608 (2) Å] and in similar rings, such as *N*-5-chlorosalicylideneaniline (2.584 Å) and 2-chloro-*N*-salicylideneaniline (2.609 Å) (Arcovito *et al.*, 1969) are shorter than the average value [2.67 (6) Å] found for similar systems in the Cambridge Structural Database [Version 5.28, updated January 2007; Allen (2002)]. This indicates the relatively strong character of the hydrogen bonding in these molecules. The two aromatic rings *A* (C9–C14) and *B* (C16–C21), connected through the azine chain, are more or less coplanar, making a dihedral angle of 10.93 (14)°. The third ring, *C* (C2–C7), is oriented out of that plane; the dihedral angle between rings *A* and *C* is 88.95 (7)°.

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Experimental

Freshly distilled salicylaldehyde (5.076 ml, 50 mmol) in ethanol (3 ml) was added dropwise to hydrazine hydrate (98%) (12.01 ml, 241 mmol) over a period of 1 h at ambient temperature; the reaction mixture was stirred vigorously during the addition. The mixture was then stirred for 10 min. The solution was cooled and the off-white solid of *N*-(aminoformimidoyl)phenol was filtered off, washed with diethyl ether and dried under vacuum. An ethanol solution (3 ml) of benzil (4.29 g, 20 mmol) was added to a solution of *N*-(aminoformimidoyl)phenol (3 g, 21.5 mmol) in ethanol (3 ml) and stirred for 3 h. The resulting light-yellow Schiff base was washed with ethanol. Crystals suitable for X-ray analysis were obtained by recrystallization from acetonitrile.

Crystal data

$C_{21}H_{16}N_2O_2$
$M_r = 328.36$
Monoclinic, $P2_1/c$
$a = 16.804$ (3) Å
$b = 9.2783$ (13) Å
$c = 11.244$ (2) Å
$\beta = 99.39$ (2)°
$V = 1729.7$ (5) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 290$ (2) K
0.5 × 0.2 × 0.1 mm

Data collection

Stoe IPDS area-detector diffractometer
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1997) $T_{min} = 0.953$, $T_{max} = 0.992$
13138 measured reflections
3356 independent reflections
1833 reflections with $I > 2\sigma(I)$
$R_{int} = 0.069$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.125$
$S = 0.89$
3356 reflections
235 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.12$ e Å^{-3}
$\Delta\rho_{min} = -0.15$ e Å^{-3}

Table 1
Selected torsion angles (°).

C8—N1—N2—C15	−164.91 (16)	N1—C8—C9—C10	169.10 (18)
N2—N1—C8—C1	3.5 (2)	N2—C15—C16—C21	−176.16 (17)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2	0.95 (3)	1.76 (3)	2.608 (2)	147 (2)

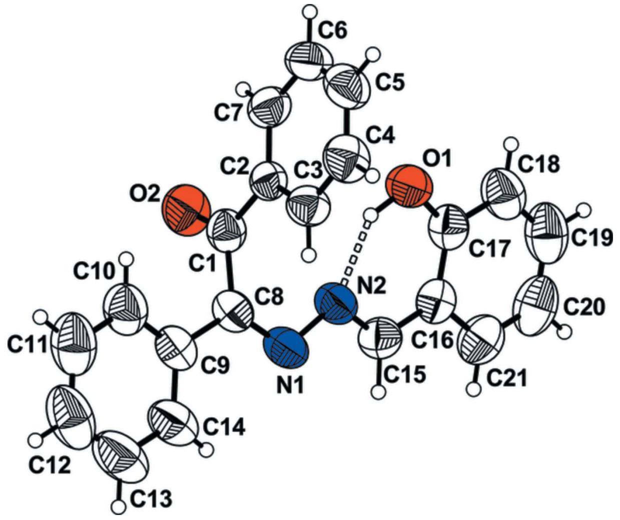

Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids for non-H atoms. The dashed line indicates a hydrogen bond.

Aromatic H atoms were placed in calculated positions (C—H = 0.93 Å) and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. Other H atoms, belonging to the hydroxyl and methylidene groups (H1 and H15), were located in difference density maps and their coordinates and isotropic displacement parameters were refined freely [O—H = 0.95 (3), C—H = 1.00 (2) Å].

Data collection: *IPDS Software* (Stoe & Cie, 1997); cell refinement: *IPDS Software*; data reduction: *IPDS Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *IPDS Software*; software used to prepare material for publication: *SHELXL97*.

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