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2,2′-{(*Z*)-Ethane-1,2-diylbis[(*Z*)-*o*-phenylenenitrilomethylidyne]}diphenol (EIEP)

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The salicylideneaniline moiety in the centrosymmetric title compound, $C_{28}H_{24}N_2O_2$, is a phenol–imine tautomer which is non-planar and photochromic. A strong intramolecular hydrogen-bonding interaction, which is a common feature in related imine–phenol compounds, stabilizes the molecular structure. The π system in the salicylideneaniline moiety interacts with symmetry-related π systems through face-to-face π–π interactions and C—H$\cdots\pi$ interactions, to stabilize the molecules in the crystal structure.

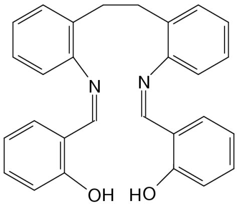
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.057
wR factor = 0.199
Data-to-parameter ratio = 21.6

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

Comment

Schiff base compounds are often used as ligands in coordination chemistry because of their ability for metal binding and, in particular, salicylaldimines are useful for the synthesis of transition metal complexes (Ligtenbarg *et al.*, 1999). *N*-Substituted salicylaldimines are 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-Mavridis *et al.*, 1978; Hadjoudis *et al.*, 1987; Xu *et al.*, 1994); charge transport occurs through intermolecular overlap of π orbitals. Of the two tautomers, one a phenol–imine structure and the other a quinoid structure, most crystal structures concern phenol–imine tautomers (Ligtenbarg *et al.*, 1999). It has been proposed that Schiff base molecules exhibiting thermochromism are planar, while those exhibiting photochromism are non-planar (Moustakali-Mavridis *et al.*, 1978).



(I)

The title compound, (I) (Fig. 1), has two salicylideneaniline moieties linked by an ethylene bridge. Only one half of the molecule constitutes the asymmetric unit and the other half is centrosymmetrically related. The crystal structure shows that the salicylideneaniline moiety is the phenol–imine tautomer with the H atom bound to O16.

The bond distances observed for the compound do not deviate significantly from the mean values for similar phenol–imine tautomeric structures (Ligtenbarg *et al.*, 1999; Elmali & Elerman, 1997; Elerman *et al.*, 1991, 1992, 1994, 1995; Elmali *et al.*, 1995; Kevran *et al.*, 1996); in particular, C9—C10 = 1.445 Å, C11—O16 = 1.349 Å and C9—N8 = 1.287 Å. The

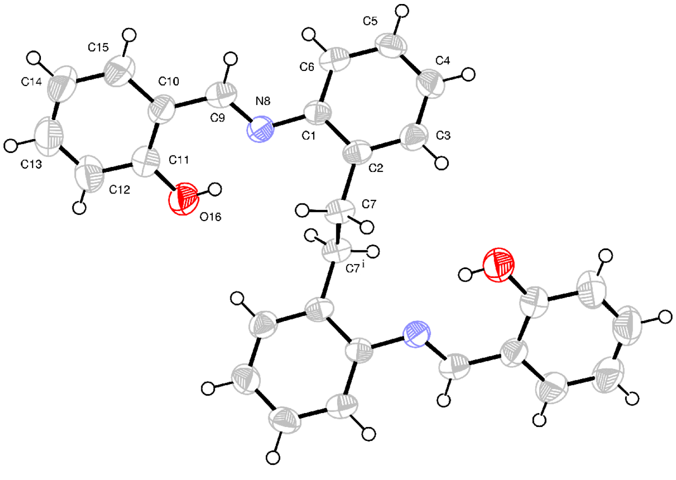


Figure 1
ORTEP-3 (Farrugia, 1997) plot of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme. [Symmetry code: (i) $2 - x, -y, -z$.]

salicylideneaniline moiety exhibits a *trans*-planar configuration of the central backbone [C1—N8—C9—C10 = 179.4 (2)°].

The salicylideneaniline moiety is non-planar and photochromic (Bernstein, 1967); moieties *A* (atoms N8/C1–C6) and *B* (O16/C9–C15) are inclined at an angle of 43.9 (1)°, reflecting mainly the twist about the N8—C9 bond [C9—N8—C1—C6 = 42.4 (3)°]. Clearly this conformation is not suitable for direct coordination to a metal ion (Elmali & Elerman, 1997).

A strong intramolecular hydrogen-bonding interaction between the imine N atom (N8) and the phenolic H atom (on O16) forms a pseudo-six-membered ring, a feature common in related imine–phenol compounds (Bhattacharyya *et al.*, 1998). The geometry of this intramolecular interaction [H16⋯N18 = 1.90 Å, O16⋯N8 = 2.616 (2) Å and O16—H16⋯N8 = 146°] is comparable to those observed for similar types of compounds (Elmali & Elerman, 1997; Elerman *et al.*, 1994, 1995; Xu *et al.*, 1994).

The phenol π system (C10–C15) of the salicylideneaniline moiety interacts with its own symmetry-related π system at $(1 - x, -y, -z)$ in a face-to-face manner, the centroid (*Cg*)–centroid distance being 3.841 (2) Å and the angle (α) between their normals being 0.02°. The benzene ring (C1–C6) also weakly interacts with its symmetry-related π system at $(2 - x, -y, 1 - z)$ [$Cg\cdots Cg$ = 4.097 (2) Å and α = 0.03°]. These interactions link the molecules into layers parallel to the *ac* plane. Atoms C5 and C15 interact with the benzene and phenol π system, respectively, of a symmetry-related molecule through C—H⋯π interactions [H5⋯*Cg*1 = 2.75 Å, C5⋯*Cg*1 = 3.569 (3) Å and C5—H5⋯*Cg*1 = 147°; H15⋯*Cg*2 = 3.33 Å, C15⋯*Cg*2 = 3.812 (3) Å and C15—H15⋯*Cg*2 = 115°; where *Cg*1 and *Cg*2 denote the centroids of rings C1–C6 and C10–C15 of the molecule at $(x, \frac{1}{2} - y, \frac{1}{2} + z)$]. These interactions link adjacent layers into a three-dimensional network (Fig. 2).

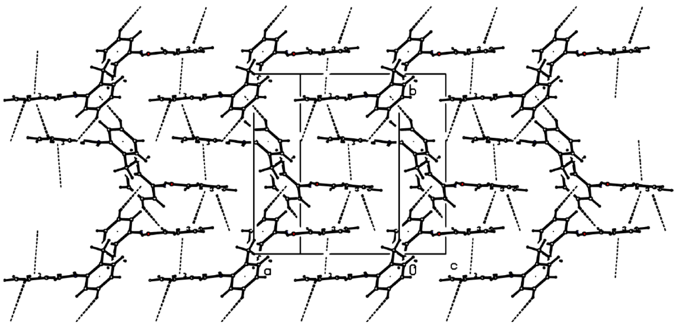


Figure 2
Packing diagram of the molecules, viewed down the *c* axis, showing the π–π and C—H⋯π interaction network (dashed lines).

Experimental

4,4′-Ethylenedianiline or 4,4′-diaminodibenzyl (1 mol, 2.12 g) in ethanol was mixed with salicyladehyde (2 mol, 2.44 g) in ethanol with vigorous stirring at room temperature (303 K). The resulting precipitate was washed with a minimum quantity of ethanol and the product was recrystallized from chloroform to give a 90% yield of the title Schiff base.

Crystal data

$C_{28}H_{24}N_2O_2$
$M_r = 420.49$
Monoclinic, $P2_1/c$
$a = 11.817$ (3) Å
$b = 13.762$ (6) Å
$c = 6.873$ (2) Å
$\beta = 101.15$ (3)°
$V = 1096.6$ (6) Å^3
$Z = 2$

$D_x = 1.273$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 8$–15°
$\mu = 0.08$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.25 × 0.22 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Non-profiled $\omega/2\theta$ scans
Absorption correction: none
3425 measured reflections
3179 independent reflections
1504 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.042$

$\theta_{\rm max} = 30.0°$
$h = -16 \rightarrow 16$
$k = 0 \rightarrow 19$
$l = 0 \rightarrow 9$
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.199$
$S = 1.01$
3179 reflections
147 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0961P)^2 + 0.0403P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.005$
$\Delta\rho_{\rm max} = 0.19$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.17$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.039 (7)

H atoms were positioned geometrically (O—H = 0.82 Å and C—H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{\rm iso}$(H) values set at $1.5U_{\rm eq}$(O) for the hydroxyl H atom and at $1.2U_{\rm eq}$(C) for the other H atoms.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEP*-3 (Farrugia, 1997); software used to prepare material for publication: *PLATON*.

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