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# (*E*)-2-Ethoxy-6-[(4-nitrophenyl)iminomethyl]phenol

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**Key indicators**

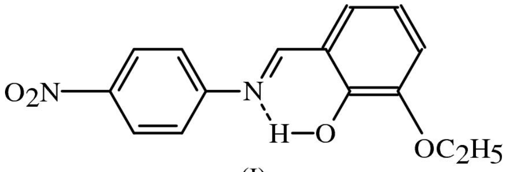
Single-crystal X-ray study
*T* = 293 K
Mean *σ*(C–C) = 0.002 Å
*R* factor = 0.035
*wR* factor = 0.068
Data-to-parameter ratio = 14.2

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

The title compound, $C_{15}H_{14}N_2O_4$, exists as an enol–imine tautomer, in which a strong intramolecular O—H···N hydrogen bond is formed. This work verifies the preference for the enol–imine tautomeric form in the solid state.

## Comment

*O*-Hydroxy Schiff bases derived from the reaction of *o*-hydroxy aldehydes with aniline have been extensively examined (Stewart & Lingafelter, 1959; Calligaris *et al.*, 1972; Maslen & Waters, 1975). Schiff base compounds display interesting photochromic and thermochromic features and can be classified by them (Cohen *et al.*, 1964; Moustakali-Mavridis *et al.*, 1980; Hadjoudis *et al.*, 1987). Photo- and thermochromism arise *via* H-atom transfer from the hydroxy O atom to the N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994).



(I)

There are two possible types of intramolecular hydrogen bonds in Schiff bases, namely keto-amine (N—H···O) and enol–imine (N···H—O) tautomeric forms. The present X-ray investigation shows that the title compound, (I), prefers the enol–imine tautomeric form rather than the keto-amine tautomeric form.

The molecular structure of (I) is shown, with the atom-numbering scheme, in Fig. 1. Selected bond lengths and angles

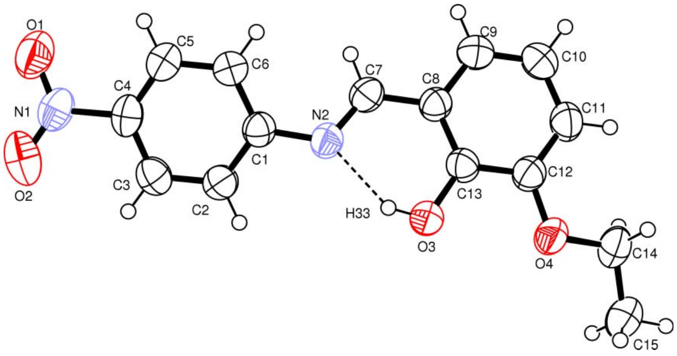


**Figure 1**
A view of the molecule of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. The dashed line indicates the intramolecular hydrogen bond.

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are listed in Table 1. The C13—O3 and C7—N2 bond lengths verify the enol–imine tautomeric form. These distances agree with the literature [1.352 (3) and 1.280 (4) Å; Karadayı *et al.*, 2003], which also show the enol–mine tautomeric form. The C4—N1 bond length in (I) is also in a good agreement with the corresponding distances in the literature [1.4671 (18) Å (Zeller & Hunter, 2004) and 1.456 (4) Å (Glidewell *et al.*, 2004)] for compounds which contain a nitro group.

As is a common feature of *o*-hydroxysalicylidene systems, compound (I) displays a strong hydrogen bond between atoms N2 and O3 (Filarowski *et al.*, 2003; Yıldız *et al.*, 1998). The bond lengths and angles of this hydrogen bond are listed in Table 2 for (I).

For a closely related compound, (*E*)-4-methoxy-6-[(4-nitrophenylimino)methyl]phenol, see Koşar *et al.* (2005).

## Experimental

Compound (I) was prepared by refluxing a mixture of a solution containing 3-ethoxysalicylaldehyde (3.5 mmol) and 4-nitroaniline (3.5 mmol) in ethanol (10 ml). The reaction mixture was stirred for 1 h under reflux and left to cool. Crystals of (I) were obtained by slow evaporation of a solution in tetrahydrofuran (yield 60%; m.p. 400–402 K).

### *Crystal data*

$C_{15}H_{14}N_2O_4$
$M_r$ = 286.28
Monoclinic, $C2/c$
$a$ = 27.883 (2) Å
$b$ = 7.1237 (7) Å
$c$ = 14.7975 (10) Å
$\beta$ = 111.524 (4)°
$V$ = 2734.2 (4) Å$^3$
$Z$ = 8

$D_x$ = 1.391 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 11318 reflections
$\theta$ = 1.5–26.1°
$\mu$ = 0.10 mm$^{-1}$
$T$ = 293 (2) K
Prism, dark red
0.42 × 0.30 × 0.11 mm

### *Data collection*

Stoe IPDS 2 diffractometer
$\omega$ rotation scans
Absorption correction: integration *X-RED32* (Stoe & Cie, 2002)
$T_{min}$ = 0.966, $T_{max}$ = 0.989
16558 measured reflections
2693 independent reflections

1289 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.071
$\theta_{max}$ = 26.0°
$h = -34 \rightarrow 34$
$k = -8 \rightarrow 8$
$l = -18 \rightarrow 17$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.069$
$S$ = 0.81
2693 reflections
190 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.075P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.08 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.14 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| N2—C7 | 1.2825 (17) | N1—O2 | 1.2197 (18) |
| C4—N1 | 1.469 (2) | N1—O1 | 1.2246 (18) |
| C13—O3 | 1.3496 (16) | | |
| O2—N1—O1 | 124.06 (18) | | |

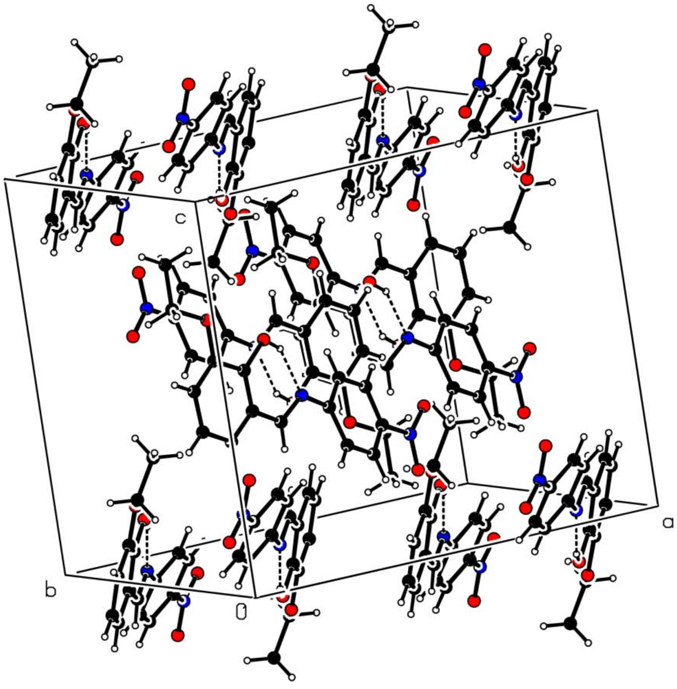

**Figure 2**
A packing diagram for (I). Dashed lines indicate intermolecular hydrogen bonds.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O3—H33···N2 | 0.82 | 1.88 | 2.6043 (16) | 147 |

All H atoms were refined using a riding model, with C—H = 0.93, 0.97 (for $CH_2$) or 0.96 Å (for $CH_3$) and O—H = 0.82 Å, and with $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(C) and 1.5$U_{eq}$(O).

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: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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