The title compound, C$_{14}$H$_{12}$N$_2$O$_2$, is stabilized in the solid state as an enol–imine tautomer, with a strong intramolecular O—H⋯N hydrogen bond, one C—H⋯N and three C—H⋯O intermolecular hydrogen bonds, generating edge-fused \(\left[ \text{S}(6)\text{R}_2(8)\text{R}_2(8)\text{R}_2(6) \right] \) motifs. The molecule is approximately planar, with a dihedral angle of 4.40 (10)° between the two aromatic rings.

Comment

Schiff bases are used as substrates in the preparation of a number of industrial and biologically active compounds via ring closure, cycloaddition and replacement reactions. Moreover, Schiff bases are also known to have biological activities, such as antimicrobial (El-Masry et al., 2000; Pandey et al., 1999), antifungal (Singh & Dash, 1988), antitumour (Hodnett & Dunn, 1970; Desai et al., 2001) and herbicidal properties (Holla et al., 2000). Schiff bases have also been employed as ligands for the complexation of metal ions (Odabas¸og˘lu et al., 2007; Aydoğan et al., 2001). On the industrial scale, they have a wide range of applications, such as dyes and pigments (Taggi et al., 2002). In continuation of our work on Schiff bases (Yathirajan et al., 2007; Odabas¸og˘lu et al., 1999, 2003, 2004, 2005a,b, 2006, 2007; Ersanlı et al., 2003), the title new Schiff base, (I), was synthesized and its crystal structure is reported (Fig. 1, Table 1).

There are two possible types of intramolecular hydrogen bonds in salicylaldehyde Schiff bases, as exhibited by the keto–amine (N⋯H—O) and enol–imine (N—H⋯O) tautomeric forms. Salicylaldehyde Schiff bases have been found in the keto form (Odabas¸og˘lu et al., 2003), in the enol form (Leardini et al., 1998; Odabas¸og˘lu et al., 2005b) and as enol/keto mixtures (Nazır et al., 2000). The present X-ray crystallographic investigation shows that compound (I) prefers the enol–imine tautonomic form.

Compound (I) displays a strong intramolecular hydrogen bond (Table 2) involving atoms N1 and O1, a common feature of salicylaldehyde systems. In (I), molecules are linked through an O—H⋯N intramolecular hydrogen bond, and molecules are...
linked through three C—H···O and one C—H···N intermolecular hydrogen bonds. These hydrogen bonds generate edge-fused \[S(6)R_2^2(8)R_2^2(8)R_1^2(6)]\] motifs (Etter, 1990) (Fig. 2 and Table 2). The molecule is almost planar, with dihedral angles of 0.47 (8°) between the Cl–C6 ring and the intramolecularly hydrogen-bonded ring, and 4.40 (10°) between the hydrogen-bonded ring and the pyridyl ring.

**Experimental**

A mixture of 5-hydroxy-2-methylisophthaldehyd (2.58 g, 0.01 mol) and pyridin-2-amine (0.94 g, 0.01 mol) in absolute ethanol (20 ml) containing two drops of 4 M sulfuric acid was refluxed for about 4 h. On cooling, the solid which separated was filtered off and recrystallized from ethanol (m.p. 393–395 K). Analysis for C_{14}H_{12}N_{2}O_{2}: found (calculated): C 69.83 (69.99), H 4.96 (5.03), N 11.52% (11.66%).

**Crystal data**

C_{14}H_{12}N_{2}O_{2}

\[\text{Mr} = 240.26\]

Monoclinic, \(P\overline{1}\)

\(a = 7.4049 (8)\) Å

\(b = 4.2957 (3)\) Å

\(c = 20.154 (2)\) Å

\(\beta = 108.847 (8)\)

\(V = 606.72 (10)\) Å³

\(Z = 2\)

Mo Kα radiation

\(\mu = 0.09\) mm⁻¹

\(T = 296\) K

0.56 \(\times\) 0.27 \(\times\) 0.18 mm

**Data collection**

Stoe IPDSII diffractometer

Absorption correction: integration

\((X-RED32;\text{ Stoe \& Cie, 2002})\)

\(T_{\text{min}} = 0.954, T_{\text{max}} = 0.989\)

10246 measured reflections

1184 independent reflections

853 reflections with \(I > 2\sigma(I)\)

\(R_{\text{int}} = 0.100\)

**Refinement**

\(R^{2} = 0.043\)

\(wR^{2} = 0.114\)

\(S = 0.99\)

1184 reflections

164 parameters

2 restraints

H-atom parameters constrained

\(\Delta \rho_{\text{max}} = 0.18\) e Å⁻³

\(\Delta \rho_{\text{min}} = -0.16\) e Å⁻³

**Table 1**

Selected geometric parameters (Å, °).

| C1—C9 | 1.432 (5) | C9—N1 | 1.282 (4) |
| C2—O1 | 1.349 (4) | C10—N1 | 1.422 (4) |
| N1—C9—C1 | 121.9 (3) | C9—N1—C10 | 120.5 (3) |
| C1—C9—N1—C10 | −177.8 (3) |

**Table 2**

Hydrogen-bond geometry (Å, °).

| D—H···A | D—H | H···A | D···A | D—H···A |
| O1—H1···N1 | 0.82 | 1.85 | 2.585 (3) | 148 |
| C9—H9···O2i | 0.93 | 2.79 | 3.620 (4) | 150 |
| C14—H14···O1i | 0.93 | 2.71 | 3.546 (5) | 151 |
| C8—H6···O2i | 0.93 | 2.77 | 3.612 (4) | 152 |
| C7—H7···N2a | 0.93 | 2.73 | 3.606 (5) | 158 |

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

In the absence of significant anomalous scattering effects, 160 Friedel pairs were merged. All H atoms were treated as riding on their parent atoms, with C—H = 0.93 Å and \(U_{\text{eq}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})\) for aromatic, aldehydeic and imino H, with C—H = 0.96 Å and \(U_{\text{eq}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})\) for methyl H, and with O—H = 0.82 Å and \(U_{\text{eq}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})\) for the H atom of the hydroxyl group.

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, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: WinGX (Farrugia, 1999).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDSII diffractometer (purchased under grant F.279 of the University Research Fund).
References
