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(*E*)-2-[1-(3-Amino-2-methylphenylimino)-ethyl]phenol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.041
wR factor = 0.114
Data-to-parameter ratio = 14.6

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

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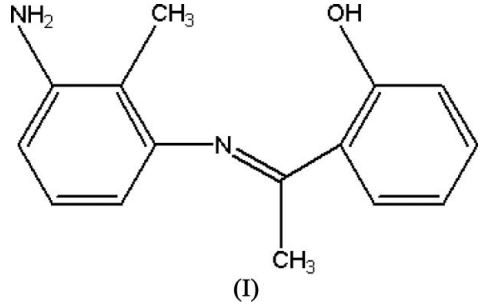
In the title compound, $C_{15}H_{16}N_2O$, the crystal packing is stabilized by intra- and intermolecular O—H···N, N—H···O and C—H···N hydrogen-bond interactions.

Comment

The synthesis of hydroxylated Schiff bases has recently attracted much attention because of their wide range of applications, including their use as catalysts for alkene epoxidation and alkane hydroxylation using sodium periodate as oxidant (Bahramian *et al.*, 2006), as carriers in the construction of a novel carbon paste electrode (CPE) and a coated wire PVC membrane electrode (CWE) for silver ions (Mashhadizadeh *et al.*, 2006), and as neutral ionophores for preparing polyvinyl chloride-based membrane sensors selective for nickel(II) (Jain et al., 2006). Moreover, the antifungal activities of Schiff bases derived from hydroxyaldehydes have been reported (Guo *et al.*, 2006). In view of the importance of this class of compounds, the title compound, (I), has been synthesized and its crystal structure is reported here.



(I)

The atom-numbering scheme adopted is shown in Fig. 1. The values of the C—C, C═C, C—O, C—N and C═N bond distances in (I) are consistent with expected values (Allen *et al.*, 1987). The angle between the planes of the two benzene rings is 62.28 (8)°. The molecules are linked through O—H···N, N—H···O and C—H···N hydrogen-bond interactions (Table 1 and Fig. 2).

Experimental

2-Hydroxyacetophenone (2.03 g, 1.8 ml, 15 mmol) and 2-methyl-1,3-pheneylenediamine (0.61 g, 5 mmol) were dissolved in warm ethanol (20 ml). The reaction mixture was refluxed for 8 h and allowed to stand. The crystals were filtered off and washed with ethanol. The pure Schiff base was recrystallized from ethanol as light-yellow crystals (m.p. 457–459 K, yield 68%). The IR spectrum showed the characteristic absorption of Schiff base C═N at 1604 cm^{-1}. The ^1H NMR spectrum showed a multiplet for aromatic protons at 6.21–7.94

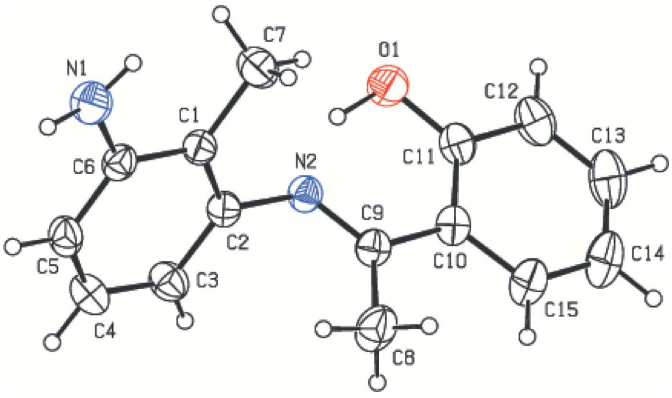


Figure 1
A view of the title compound, (I), showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

p.p.m. The OH group appeared as a singlet at 14.57 p.p.m. The ^{13}C NMR spectrum showed C═N at 171.23 p.p.m. The mass spectrum showed the molecular ion at *m*/*e* 240.

Crystal data

$C_{15}H_{16}N_2O$
M_r = 240.30
Monoclinic, $P2_1/c$
a = 11.6558 (7) Å
b = 7.9917 (6) Å
c = 16.0978 (10) Å
β = 118.619 (4)°
V = 1316.30 (16) Å^3
Z = 4
D_x = 1.213 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
Prism, light yellow
0.55 × 0.46 × 0.39 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: none
17381 measured reflections
2583 independent reflections
2097 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.114
S = 1.06
2583 reflections
177 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 0.1559P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	1.04 (2)	1.54 (2)	2.4987 (18)	150.4 (15)
N1—H1A···O1^{i}	0.94 (2)	2.118 (19)	3.042 (2)	169.4 (17)
N1—H1B···O1^{ii}	0.91 (2)	2.50 (2)	3.270 (2)	142.8 (14)
C7—H7A···N2	0.96	2.41	2.858 (2)	108

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$.

H atoms bound to the N and O atoms were found in a difference Fourier map and refined freely. Other H atoms were placed in calculated positions, with C—H = 0.93–0.96 Å and refined in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

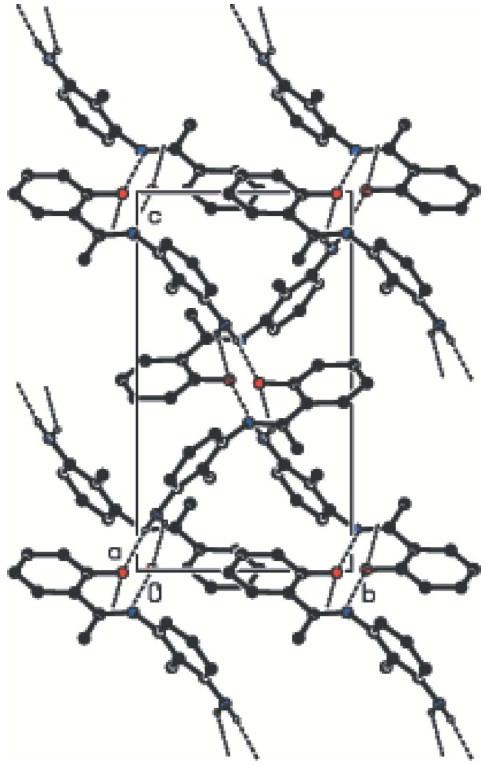


Figure 2
The crystal packing of (I), viewed along the *a* axis, showing the hydrogen-bonding interactions (dashed lines). H atoms have been omitted.

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: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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