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2-(*o*-Tolyliminomethyl)phenol

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.142
Data-to-parameter ratio = 17.4

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

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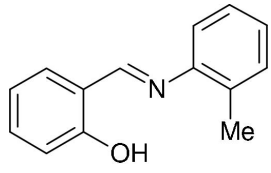
The molecule of the title compound, $C_{14}H_{13}NO$, is roughly planar and displays a *trans* configuration with respect to the C=N double bond.

Comment

Schiff base compounds have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. As an extension of our work on the structural characterization of Schiff base compounds, the crystal structure of the title compound, (I), is reported here.



(I)

In the title compound, (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). The C7=N1 bond length of 1.274 (2) Å conforms to the value for a double bond. The molecule is roughly planar and displays a *trans* configuration with respect to the C7=N1 double bond. The dihedral angle between the two benzene rings is 2.6 (2)°. A strong O—H···N intramolecular hydrogen-bond interaction is observed (Table 1).

Experimental

o-Toluidine and salicylaldehyde were available commercially and were used without further purification. *o*-Toluidine (2.0 mmol, 214 mg) and salicylaldehyde (2.0 mmol, 244 mg) were dissolved in

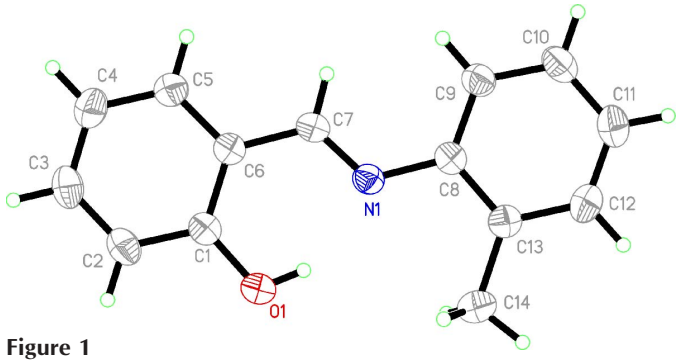


Figure 1
The structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

methanol (100 ml). The mixture was stirred at room temperature for 1 h to give a clear yellow solution. After keeping the solution in air for 10 d, yellow block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvent. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using P_4O_{10} (yield 85.7%). Analysis found: C 79.5, H 6.2, N 6.6%; calculated for $C_{14}H_{13}NO$: C 79.6, H 6.2, N 6.6%.

Crystal data

$C_{14}H_{13}NO$	D_x = 1.244 Mg m^{-3}
M_r = 211.25	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 878 reflections
a = 4.693 (1) Å	θ = 2.7–21.8°
b = 19.140 (3) Å	μ = 0.08 mm^{-1}
c = 12.682 (2) Å	T = 298 (2) K
β = 97.973 (2)°	Block, yellow
V = 1128.2 (3) Å^3	0.20 × 0.20 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2558 independent reflections
	1563 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.040
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 27.5°
	$h = -6 \rightarrow 6$
T_{min} = 0.984, T_{max} = 0.992	$k = -24 \rightarrow 24$
12565 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + 0.2156P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.057	
$wR(F^2)$ = 0.142	
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
2558 reflections	$\Delta\rho_{max}$ = 0.12 e Å^{-3}
147 parameters	$\Delta\rho_{min}$ = −0.15 e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.88	2.6104 (19)	148

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.96 Å and an O—H distance of 0.82 Å, and with U_{iso}(H) = 1.2 or 1.5U_{eq}(C/O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

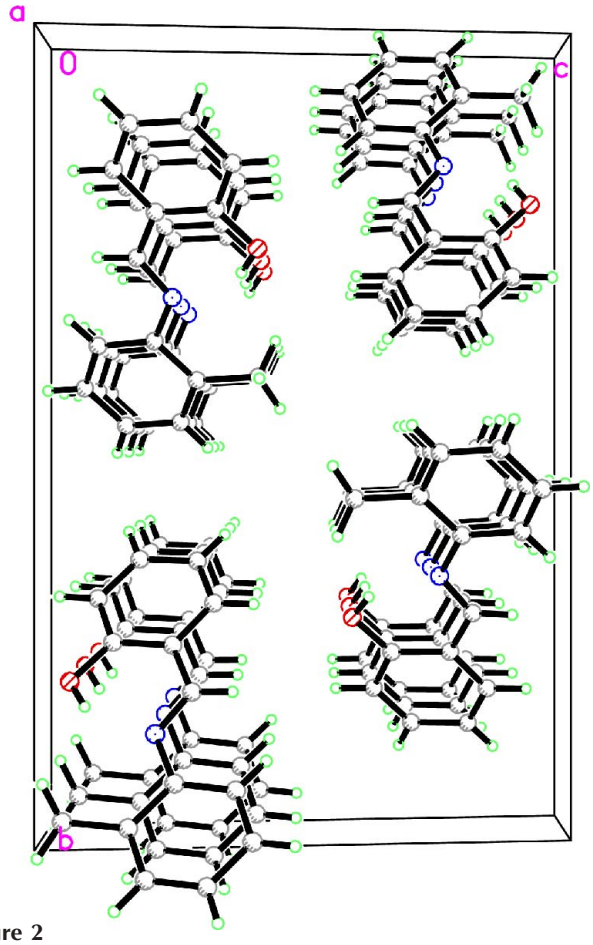


Figure 2
The crystal packing of (I), viewed along the *a* axis.

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