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4-Chloro-2-(*p*-tolyliminomethyl)phenol

Xin-Li Zhang and Zong-Xiao Li*

Department of Chemistry, Baoji University of Arts and Science, Baoji, Shaanxi 721007, People's Republic of China

Correspondence e-mail: mingtian8001@163.com

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The title compound, $C_{14}H_{12}ClNO$, is a Schiff base compound, derived from the condensation of 5-chlorosalicylaldehyde and *p*-methoxybenzenamine in MeOH. The two benzene rings are linked by a C=N bond and form a dihedral angle of 44.4 (2)°.

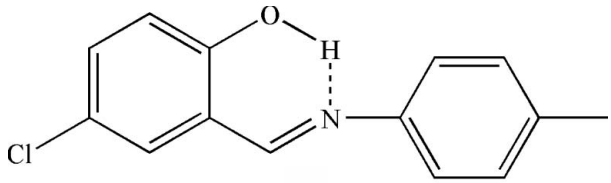
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.037
wR factor = 0.099
Data-to-parameter ratio = 9.9

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

Comment

As an extension of our work on the structural characterization of Schiff base compounds (Li & Zhang, 2004*a*,*b*, 2005; Zhang & Li, 2005), the crystal structure of the title compound, (I), is reported here



(I)

In Schiff base compound (I) (Fig. 1), all the bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and are comparable to those observed in a similar Schiff base compound (Kennedy & Reglinski, 2001). The two benzene rings are linked by a C=N bond and form a dihedral angle of 44.4 (2). The N1—C1—C2—C3, C1—N1—C2—C7, C1—N1—C8—C13 and C1—N1—C8—C9 torsion angles are −6.1 (6) and 179.8 (3)°, and 149.4 (3) and −35.9 (6)°, respectively. Atoms O1 and Cl1 deviate from the benzene ring mean plane by −0.010 (6) and 0.137 Å, respectively. The compound is supported by an intramolecular O—H···N hydrogen bond (Table 1). The C1=N1 bond length [1.273 (5) Å] confirms it to be a double bond. As expected, the molecule adopts a *trans* configuration about the C=N bond.

Experimental

5-Chlorosalicylaldehyde (0.1 mmol, 15.7 mg) and *p*-toluidine (0.1 mmol, 10.7 mg) were dissolved in methanol (10 ml). The mixture was stirred at room temperature for about 30 min to give a clear yellow solution. After leaving the solution to stand in air for 12 d, yellow block-shaped crystals formed. The crystals were isolated by filtration, washed with methanol and dried in a vacuum desiccator using anhydrous $CaCl_2$ (yield 54%). Elemental analysis found: C 68.3, H 4.8%; calculated for $C_{14}H_{12}ClNO$: C 68.4, H 4.9%.

Crystal data

$C_{14}H_{12}ClNO$
$M_r = 245.70$
Monoclinic, *Pc*
$a = 13.846\ (11)$ Å
$b = 6.986\ (6)$ Å
$c = 6.176\ (5)$ Å
$\beta = 96.363\ (10)^\circ$
$V = 593.7\ (8)$ Å^3
$Z = 2$
$D_x = 1.374$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.30$ mm^{-1}
$T = 298\ (2)$ K
Block, yellow
$0.42 \times 0.25 \times 0.10$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.883$, $T_{max} = 0.970$
2956 measured reflections
1531 independent reflections
1195 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.099$
$S = 1.02$
1531 reflections
154 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.04P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}
Absolute structure: Flack (1983), 484 Friedel pairs
Flack parameter: 0.000 (2)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*.

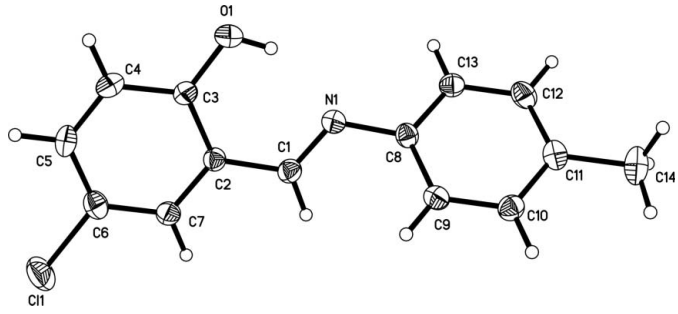


Figure 1
The molecular structure of the title compound with 30% probability displacement ellipsoids.

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