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# 2-[(*E*)-(5-Chloro-2-methylphenyl)iminomethyl]-4-methylphenol

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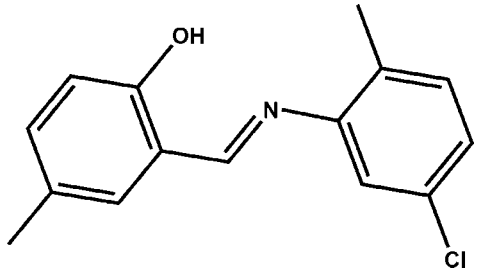
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.041; $wR$ factor = 0.100; data-to-parameter ratio = 14.1.

In the molecule of the title Schiff base compound, $C_{15}H_{14}ClNO$, the two benzene rings are twisted with respect to each other, with a dihedral angle of 35.0 (3)°; an intramolecular O—H···N hydrogen bond occurs. In the crystal, weak C—H···$\pi$ interactions between methyl groups and chlorophenyl rings link the molecules into supramolecular chains running along the *a* axis.

## Related literature

For background to phyenylamine compounds, see: Fan *et al.* (2012). For applications of Schiff base derivatives, see: Siddiqui *et al.* (2006); Ebrahimipour *et al.* (2012).




## Experimental

### Crystal data

$C_{15}H_{14}ClNO$
$M_r$ = 259.72
Orthorhombic, $P2_12_12_1$
$a$ = 7.6629 (10) Å
$b$ = 11.8442 (14) Å
$c$ = 14.342 (2) Å
$V$ = 1301.7 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 293 K
0.45 × 0.42 × 0.35 mm

### Data collection

Agilent Xcalibur Gemini ultra diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.88, $T_{max}$ = 0.91
8663 measured reflections
2382 independent reflections
1769 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
$S$ = 1.03
2382 reflections
169 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Absolute structure: Flack (1983), with 991 Friedel pairs
Absolute structure parameter: −0.18 (9)

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

*Cg*1 is the centroid of the C9–C14 benzene ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.84 (4) | 1.84 (4) | 2.629 (3) | 154 (4) |
| C7—H7*C*···*Cg*1$^{i}$ | 0.96 | 2.91 | 3.767 (3) | 149 |

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{5}{2}, -z+1$.

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The author acknowledges Lishui University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5720).

## References

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# supporting information

*Acta Cryst.* (2013). E**69**, o1349 [doi:10.1107/S1600536813019454]

## 2-[(*E*)-(5-Chloro-2-methylphenyl)iminomethyl]-4-methylphenol

**Yun-Fa Zheng**

### S1. Comment

Phyenylamine group has received attention in recent years for their unique physical and chemical properties (Fan *et al.*, 2012). On the other hand, Schiff bases derived from salicyladehyde and methylaniline with varous substituents have exhibited potential application in pharmaceutical field for their properties of antitumor, antimicrobial and antiviral activities (Siddiqui *et al.*, 2006). Moreover, Schiff bases ligands are potentially capable of forming stable complexes by coordination of metal ions with their nitrogen donors (Ebrahimipour *et al.*, 2012). As an extension work on the structural characterization of Schiff base compounds, the title compound is reported.

The molecular structure of title compound shows an E configuration, with a C9—N1═C8—C6 torsion angle of 0.26 (4)°. The bond distance of N1═C8 at 1.284 (3)Å is a typical double bond. It is noteworthy that H1 atom bonded to O1 is involved in an O1—H1···N1 intramolecular hydrogen bond, which results in formation of a six-membered ring (Fig. 1). The dihedral angle between the two planes of the chlorophyenyl ring and methylphenol ring is 35.0 (3)°.

### S2. Experimental

A mixture of 5-chloro-2-methylaniline (1.42g, 10.0 mmol), 3-methyl-2-hydroxybenzaldehyde (1.36g, 10.0 mmol) in 50.0 ml $CH_2Cl_2$ was fluxed under an Ar atmosphere for about 6 h to gain a yellow precipitate. The product was collected by filtration and washed with cold ethanol to give the Schiff base compound (2.25g in 86% yield). The yellow single crystals suitable for X-ray analysis were crystallized from $CH_2Cl_2$/absolute ethanol (3/2) systems by slow evaporation of solvents at room temperature over a week. Elemental analysis. Calc. for $C_{15}H_{14}ClNO$: C 69.36, H, 6.43%; Found C 69.92, H 6.80%.

### S3. Refinement

Hydroxy H atom was located in a difference Fourier map and positional parameters were refined freely, $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were fixed geometrically and treated as riding with C—H = 0.96 Å (methyl) or 0.93 Å (aromatic), $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms or $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms.

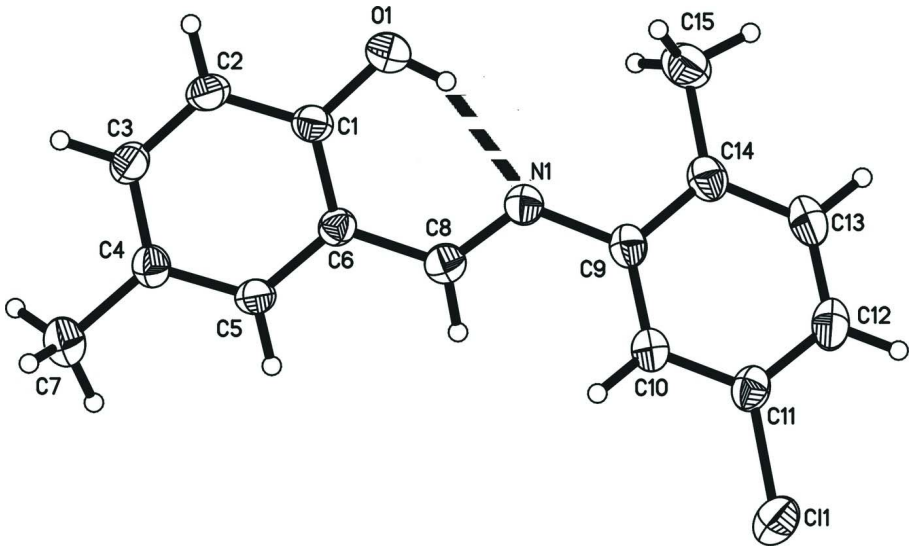


**Figure 1**

Thermal ellipsoid plot of the title compound. Ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radius. The dashed line indicates the intramolecular hydrogen bond.

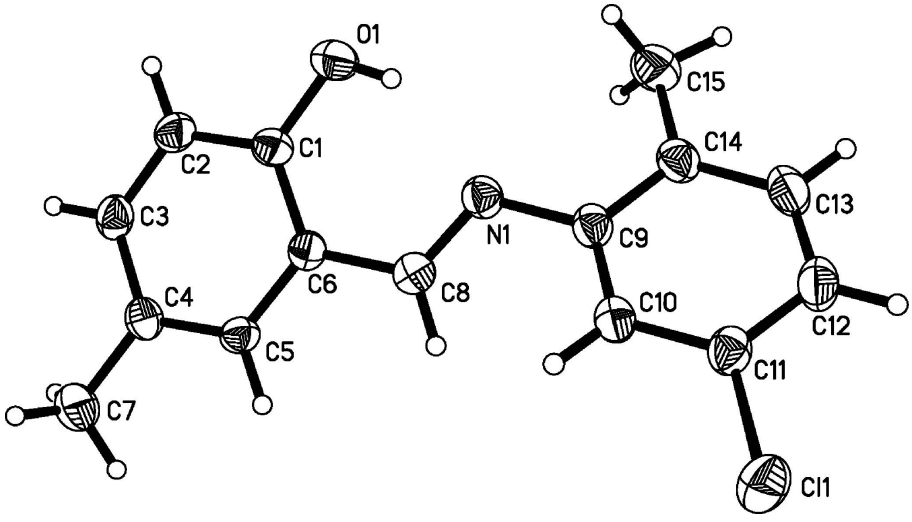


**Figure 2**

Thermal ellipsoid plot of the title compound. Ellipsoids are drawn at the 50% probability level and H atoms are represented as small spheres of arbitrary radius.

**2-[(*E*)-(5-Chloro-2-methylphenyl)iminomethyl]-4-methylphenol**

*Crystal data*

$C_{15}H_{14}ClNO$
$M_r = 259.72$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 7.6629$ (10) Å
$b = 11.8442$ (14) Å
$c = 14.342$ (2) Å
$V = 1301.7$ (3) Å$^3$
$Z = 4$
$F(000) = 544$
$D_x = 1.325$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1894 reflections
$\theta = 3.4$–$29.6°$

$\mu$ = 0.28 mm$^{-1}$
$T$ = 293 K

Block, yellow
0.45 × 0.42 × 0.35 mm

*Data collection*

Agilent Xcalibur Gemini ultra diffractometer with Atlas detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.3592 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
$T_{min}$ = 0.88, $T_{max}$ = 0.91

8663 measured reflections
2382 independent reflections
1769 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.048
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 3.4°
$h$ = −9→7
$k$ = −14→14
$l$ = −15→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.100
$S$ = 1.03
2382 reflections
169 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0463P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.024 (2)
Absolute structure: Flack (1983), with 991 Friedel pairs
Absolute structure parameter: −0.18 (9)

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted R-factor wR and goodness of fit S are based on $F^2$, conventional R-factors R are based on F, with F set to zero for negative $F^2$. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on $F^2$ are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.87007 (10) | 0.98698 (7) | 0.87968 (5) | 0.0705 (3) |
| O1 | 1.1714 (3) | 1.01909 (17) | 0.36679 (14) | 0.0651 (6) |
| N1 | 1.0171 (3) | 0.99976 (18) | 0.52972 (14) | 0.0456 (5) |
| C1 | 1.1228 (3) | 1.1295 (2) | 0.36948 (19) | 0.0449 (6) |
| C2 | 1.1680 (4) | 1.1989 (2) | 0.2958 (2) | 0.0510 (7) |
| H2 | 1.2327 | 1.1705 | 0.2462 | 0.061* |
| C3 | 1.1167 (4) | 1.3109 (2) | 0.29627 (19) | 0.0498 (7) |
| H3 | 1.1449 | 1.3561 | 0.2454 | 0.060* |
| C4 | 1.0248 (3) | 1.3579 (2) | 0.36974 (19) | 0.0451 (7) |
| C5 | 0.9829 (3) | 1.2883 (2) | 0.44320 (19) | 0.0421 (6) |

| | | | | |
|---|---|---|---|---|
| H5 | 0.9215 | 1.3181 | 0.4934 | 0.050* |
| C6 | 1.0296 (3) | 1.1738 (2) | 0.44475 (18) | 0.0395 (6) |
| C7 | 0.9729 (4) | 1.4803 (2) | 0.3692 (2) | 0.0653 (8) |
| H7A | 0.8860 | 1.4932 | 0.4162 | 0.098* |
| H7B | 0.9261 | 1.4996 | 0.3092 | 0.098* |
| H7C | 1.0733 | 1.5263 | 0.3818 | 0.098* |
| C8 | 0.9758 (3) | 1.1045 (2) | 0.52278 (19) | 0.0458 (7) |
| H8 | 0.9087 | 1.1370 | 0.5697 | 0.055* |
| C9 | 0.9585 (3) | 0.9368 (2) | 0.6085 (2) | 0.0446 (7) |
| C10 | 0.9508 (3) | 0.9850 (2) | 0.69650 (18) | 0.0459 (6) |
| H10 | 0.9883 | 1.0589 | 0.7055 | 0.055* |
| C11 | 0.8874 (4) | 0.9232 (2) | 0.77061 (19) | 0.0493 (7) |
| C12 | 0.8366 (4) | 0.8127 (3) | 0.7589 (2) | 0.0596 (8) |
| H12 | 0.7943 | 0.7710 | 0.8089 | 0.071* |
| C13 | 0.8498 (4) | 0.7652 (2) | 0.6719 (2) | 0.0593 (8) |
| H13 | 0.8168 | 0.6901 | 0.6644 | 0.071* |
| C14 | 0.9102 (3) | 0.8243 (2) | 0.5945 (2) | 0.0503 (7) |
| C15 | 0.9174 (4) | 0.7697 (2) | 0.5002 (2) | 0.0680 (9) |
| H15A | 1.0351 | 0.7715 | 0.4773 | 0.102* |
| H15B | 0.8427 | 0.8099 | 0.4579 | 0.102* |
| H15C | 0.8791 | 0.6927 | 0.5050 | 0.102* |
| H1 | 1.136 (5) | 0.993 (3) | 0.418 (3) | 0.102* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0837 (5) | 0.0789 (6) | 0.0487 (5) | 0.0012 (4) | 0.0059 (4) | 0.0083 (4) |
| O1 | 0.0850 (14) | 0.0494 (12) | 0.0608 (14) | 0.0107 (11) | 0.0181 (11) | −0.0039 (11) |
| N1 | 0.0509 (12) | 0.0429 (12) | 0.0430 (13) | −0.0007 (12) | −0.0008 (10) | 0.0014 (11) |
| C1 | 0.0489 (14) | 0.0421 (14) | 0.0439 (17) | −0.0003 (12) | 0.0010 (14) | −0.0065 (13) |
| C2 | 0.0581 (17) | 0.0534 (17) | 0.0414 (16) | −0.0070 (14) | 0.0103 (14) | −0.0092 (14) |
| C3 | 0.0590 (16) | 0.0519 (16) | 0.0386 (16) | −0.0127 (16) | 0.0026 (14) | 0.0014 (13) |
| C4 | 0.0463 (14) | 0.0429 (14) | 0.0460 (18) | −0.0033 (12) | −0.0052 (13) | 0.0036 (13) |
| C5 | 0.0442 (14) | 0.0442 (14) | 0.0378 (16) | −0.0006 (12) | 0.0034 (12) | −0.0058 (12) |
| C6 | 0.0409 (13) | 0.0416 (14) | 0.0360 (16) | −0.0039 (12) | −0.0008 (12) | −0.0009 (12) |
| C7 | 0.0764 (19) | 0.0512 (16) | 0.068 (2) | 0.0039 (16) | 0.0027 (17) | 0.0091 (17) |
| C8 | 0.0445 (15) | 0.0480 (15) | 0.0447 (18) | −0.0003 (13) | 0.0003 (13) | −0.0012 (13) |
| C9 | 0.0411 (14) | 0.0421 (14) | 0.0505 (19) | 0.0006 (11) | −0.0003 (13) | 0.0066 (13) |
| C10 | 0.0464 (14) | 0.0417 (13) | 0.0497 (17) | −0.0017 (13) | −0.0003 (12) | 0.0056 (14) |
| C11 | 0.0475 (16) | 0.0528 (16) | 0.0475 (18) | 0.0044 (14) | 0.0002 (14) | 0.0111 (13) |
| C12 | 0.0596 (19) | 0.0546 (19) | 0.064 (2) | −0.0002 (15) | 0.0067 (15) | 0.0199 (16) |
| C13 | 0.0618 (19) | 0.0399 (15) | 0.076 (2) | −0.0021 (14) | 0.0013 (17) | 0.0095 (16) |
| C14 | 0.0469 (16) | 0.0437 (15) | 0.060 (2) | 0.0048 (13) | −0.0010 (14) | 0.0052 (14) |
| C15 | 0.075 (2) | 0.0530 (17) | 0.076 (2) | −0.0040 (16) | 0.0029 (17) | −0.0109 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C11 | 1.742 (3) | C7—H7B | 0.9600 |
| O1—C1 | 1.361 (3) | C7—H7C | 0.9600 |
| O1—H1 | 0.84 (4) | C8—H8 | 0.9300 |
| N1—C8 | 1.284 (3) | C9—C10 | 1.387 (4) |
| N1—C9 | 1.426 (3) | C9—C14 | 1.397 (3) |
| C1—C2 | 1.383 (4) | C10—C11 | 1.379 (3) |
| C1—C6 | 1.396 (3) | C10—H10 | 0.9300 |
| C2—C3 | 1.383 (4) | C11—C12 | 1.376 (4) |
| C2—H2 | 0.9300 | C12—C13 | 1.372 (4) |
| C3—C4 | 1.384 (4) | C12—H12 | 0.9300 |
| C3—H3 | 0.9300 | C13—C14 | 1.392 (4) |
| C4—C5 | 1.376 (3) | C13—H13 | 0.9300 |
| C4—C7 | 1.503 (4) | C14—C15 | 1.501 (4) |
| C5—C6 | 1.403 (3) | C15—H15A | 0.9600 |
| C5—H5 | 0.9300 | C15—H15B | 0.9600 |
| C6—C8 | 1.448 (3) | C15—H15C | 0.9600 |
| C7—H7A | 0.9600 | | |

| | | | |
|---|---|---|---|
| C1—O1—H1 | 104 (3) | N1—C8—H8 | 118.8 |
| C8—N1—C9 | 119.3 (2) | C6—C8—H8 | 118.8 |
| O1—C1—C2 | 118.8 (2) | C10—C9—C14 | 120.8 (2) |
| O1—C1—C6 | 121.5 (2) | C10—C9—N1 | 121.2 (2) |
| C2—C1—C6 | 119.7 (2) | C14—C9—N1 | 117.9 (2) |
| C1—C2—C3 | 119.7 (3) | C11—C10—C9 | 119.8 (2) |
| C1—C2—H2 | 120.2 | C11—C10—H10 | 120.1 |
| C3—C2—H2 | 120.2 | C9—C10—H10 | 120.1 |
| C2—C3—C4 | 122.3 (2) | C12—C11—C10 | 120.7 (3) |
| C2—C3—H3 | 118.9 | C12—C11—Cl1 | 120.1 (2) |
| C4—C3—H3 | 118.9 | C10—C11—Cl1 | 119.3 (2) |
| C5—C4—C3 | 117.4 (2) | C13—C12—C11 | 118.7 (3) |
| C5—C4—C7 | 121.3 (2) | C13—C12—H12 | 120.6 |
| C3—C4—C7 | 121.3 (2) | C11—C12—H12 | 120.6 |
| C4—C5—C6 | 122.1 (2) | C12—C13—C14 | 122.9 (3) |
| C4—C5—H5 | 118.9 | C12—C13—H13 | 118.6 |
| C6—C5—H5 | 118.9 | C14—C13—H13 | 118.6 |
| C1—C6—C5 | 118.7 (2) | C13—C14—C9 | 117.0 (3) |
| C1—C6—C8 | 122.1 (2) | C13—C14—C15 | 121.0 (2) |
| C5—C6—C8 | 119.2 (2) | C9—C14—C15 | 122.0 (3) |
| C4—C7—H7A | 109.5 | C14—C15—H15A | 109.5 |
| C4—C7—H7B | 109.5 | C14—C15—H15B | 109.5 |
| H7A—C7—H7B | 109.5 | H15A—C15—H15B | 109.5 |
| C4—C7—H7C | 109.5 | C14—C15—H15C | 109.5 |
| H7A—C7—H7C | 109.5 | H15A—C15—H15C | 109.5 |
| H7B—C7—H7C | 109.5 | H15B—C15—H15C | 109.5 |
| N1—C8—C6 | 122.5 (2) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C9–C14 benzene ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.84 (4) | 1.84 (4) | 2.629 (3) | 154 (4) |
| C7—H7*C*···*Cg*1$^{i}$ | 0.96 | 2.91 | 3.767 (3) | 149 |

Symmetry code: (i) *x*+1/2, −*y*+5/2, −*z*+1.