Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-[(*E*)-(2-Chlorophenyl)iminomethyl]-6-methylphenol

Peihua Zhu,* Jiemei Yu, Hongyan Wang, Chunlai Zhang and Dongming Yang

School of Chemistry and Chemical Engineering, University of Jinan, Jinan 250022, People's Republic of China
Correspondence e-mail: chm_zhuph@ujn.edu.cn

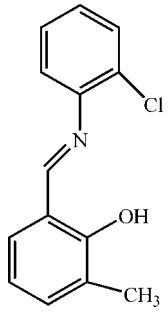
Received 18 August 2010; accepted 23 August 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.096; data-to-parameter ratio = 15.7.

The title compound, $C_{14}H_{12}ClNO$, a Schiff base derived from 3-methylsalicylaldehyde, crystallizes in the phenol–imine tautomeric form with an *E* conformation for the imine functionality. The molecule is not planar, the dihedral angle between the aromatic rings being 36.38 (5)°. The hydroxy H atom is involved in a strong intramolecular O—H···N hydrogen bond, generating an *S*(6) ring.

Related literature

For background information and applications of Schiff base complexes, see: Barton & Ollis (1979); Layer (1963); Ingold (1969); Cohen *et al.* (1964); Henrici-Olive & Olive (1984); Garnovskii *et al.* (1993). For related structures, see: Köysal *et al.* (2007); Kılıç *et al.* (2009); Şahin *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{12}ClNO$
M_r = 245.70
Orthorhombic, $P2_12_12_1$
a = 7.8318 (14) Å
b = 11.693 (2) Å
c = 13.250 (2) Å
V = 1213.4 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 293 K
0.21 × 0.11 × 0.06 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.940, T_{max} = 0.982
6803 measured reflections
2477 independent reflections
1486 reflections with $I > 2\sigma(I)$
R_{int} = 0.070

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.096
S = 1.00
2477 reflections
158 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: Flack (1983), 1034 Friedel pairs
Flack parameter: −0.06 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.87 (1)	1.84 (2)	2.615 (3)	148 (3)

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by Shandong Province (2007BS02016).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2056).

References

Barton, D. & Ollis, W. D. (1979). *Comprehensive Organic Chemistry*, Vol 2. Oxford: Pergamon Press.
Bruker (2001). *SAINT-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2004). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cohen, M. D., Schmidt, G. M. J. & Flavian, S. (1964). *J. Chem. Soc.* pp. 2041–2051.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Garnovskii, A. D., Nivorozhkin, A. L. & Minkin, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Henrici-Olive, G. & Olive, S. (1984). *The Chemistry of the Catalyzed Hydrogenation of Carbon Monoxide*. Berlin: Springer.
Ingold, C. K. (1969). *Structure and Mechanism in Organic Chemistry*, 2nd ed. Ithaca: Cornell University Press.
Kılıç, I., Işık, Ş., Ağar, E. & Erşahin, F. (2009). *Acta Cryst.* E**65**, o1347.
Köysal, Y., Işık, Ş. & Ağar, A. (2007). *Acta Cryst.* E**63**, o4916.
Layer, R. W. (1963). *Chem. Rev.* **63**, 489–510.
Şahin, Z. S., Işık, Ş., Erşahin, F. & Ağar, E.(2009). *Acta Cryst.* E**65**, o811.
Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

supplementary materials

Acta Cryst. (2010). E**66**, o2460 [**doi:10.1107/S1600536810033969**]

2-[(*E*)-(2-Chlorophenyl)iminomethyl]-6-methylphenol

P. Zhu, J. Yu, H. Wang, C. Zhang and D. Yang

Comment

Schiff bases are used as starting materials in the synthesis of important drugs (Layer, 1963; Ingold, 1969). A large number of Schiff bases and their complexes have been studied for their interesting and important properties, *e.g.* catalytic activity (Henrici-Olive & Olive, 1984), photochromic properties (Cohen *et al.*, 1964), biological activity (Barton *et al.*, 1979). On the other hand, Schiff base ligands play a vital role in coordination chemistry due to their metal binding ability (Garnovskii *et al.*, 1993).

The structure of the title compound is shown in Fig. 1. The C7═N1 double bond of 1.283 (3) Å is slightly longer than the literature values found in similar structures (Köysal *et al.*, 2007; Kılıç *et al.,* 2009; Şahin *et al.,* 2009) in the range of 1.262 (8)-1.279 (3) Å. The title molecule is not planar with a dihedral angle between the aromatic rings C1/C6 and C8/C13 of 36.38 (5) °. The imino group is coplanar with the hydroxyphenyl ring with the torsion angle C13—C8—C7—N1 of 1.6 (4) °.

The molecular structure is stabilized by a strong intramolecular O—H···N hydrogen bond.

Experimental

A solution of 3-methylsalicylaldehyde (0.0681 g, 0.5 mmol) in ethanol (10 ml) was added to a solution of 2-chlorobenzenamine (0.0638 g, 0.5 mmol) in ethanol (20 ml). The reaction mixture was stirred for 2 h under reflux. Single crystals suitable for a X-ray analysis were obtained from ethanol by slow evaporation (0.0749 g, 61%).

Refinement

The H atom bounded to O1 was located in the difference Fourier map and freely refined with U_{iso}(H) = 1.2U_{eq} (O). All other H atoms were placed in calculated positions and refined using a riding-model approximation with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H atoms, and with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms.

Figures

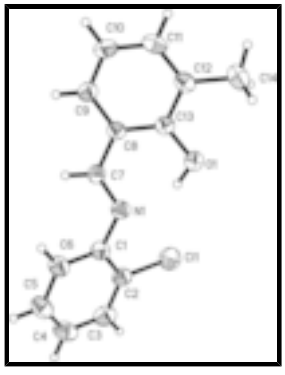


Fig. 1. The molecular structure of the title compound, with the atom-numbering scheme and 25% probability displacement ellipsoids for the non-H atoms.

2-[(*E*)-(2-Chlorophenyl)iminomethyl]-6-methylphenol

Crystal data

$C_{14}H_{12}ClNO$	$F(000) = 512$
$M_r = 245.70$	$D_x = 1.345$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 1163 reflections
$a = 7.8318$ (14) Å	$\theta = 3.1$–$28.8°$
$b = 11.693$ (2) Å	$\mu = 0.30$ mm^{-1}
$c = 13.250$ (2) Å	$T = 293$ K
$V = 1213.4$ (4) Å^3	Needle, yellow
$Z = 4$	0.21 × 0.11 × 0.06 mm

Data collection

Bruker APEXII CCD area-detector diffractometer	2477 independent reflections
Radiation source: fine-focus sealed tube	1486 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.070$
φ and ω scans	$\theta_{max} = 26.4°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)	$h = -9\rightarrow9$
$T_{min} = 0.940$, $T_{max} = 0.982$	$k = -14\rightarrow14$
6803 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.051$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0358P)^2 + 0.0414P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
2477 reflections	$\Delta\rho_{max} = 0.15$ e Å^{-3}
158 parameters	$\Delta\rho_{min} = -0.14$ e Å^{-3}
1 restraint	Absolute structure: Flack (1983), 1034 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: −0.06 (9)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations

between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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	−0.30427 (11)	−0.84282 (9)	−0.18201 (8)	0.0873 (3)
C11	−0.2023 (4)	−0.5269 (3)	−0.6436 (3)	0.0609 (9)
H11	−0.1358	−0.4949	−0.6945	0.073*
C2	−0.6147 (5)	−0.8244 (3)	−0.0959 (3)	0.0673 (9)
H2	−0.5727	−0.8740	−0.0469	0.081*
C4	−0.8405 (4)	−0.7124 (3)	−0.1622 (3)	0.0704 (10)
H4	−0.9518	−0.6851	−0.1577	0.085*
C13	−0.2304 (4)	−0.5959 (2)	−0.4763 (2)	0.0460 (7)
N1	−0.4592 (3)	−0.68266 (18)	−0.32559 (19)	0.0510 (6)
C8	−0.4038 (3)	−0.6210 (2)	−0.4942 (2)	0.0446 (7)
C5	−0.7384 (3)	−0.6793 (3)	−0.2418 (3)	0.0600 (8)
H5	−0.7817	−0.6305	−0.2910	0.072*
C1	−0.5125 (4)	−0.7905 (2)	−0.1741 (2)	0.0546 (8)
C3	−0.7793 (5)	−0.7849 (3)	−0.0899 (3)	0.0726 (10)
H3	−0.8492	−0.8075	−0.0368	0.087*
C9	−0.4702 (4)	−0.5986 (2)	−0.5894 (2)	0.0568 (8)
H9	−0.5835	−0.6167	−0.6030	0.068*
C7	−0.5128 (3)	−0.6658 (2)	−0.4159 (2)	0.0476 (7)
H7	−0.6257	−0.6830	−0.4313	0.057*
C12	−0.1285 (3)	−0.5488 (2)	−0.5514 (2)	0.0509 (8)
C6	−0.5706 (3)	−0.7186 (2)	−0.2491 (2)	0.0495 (7)
C10	−0.3721 (4)	−0.5507 (3)	−0.6631 (2)	0.0638 (9)
H10	−0.4190	−0.5342	−0.7260	0.077*
C14	0.0568 (4)	−0.5250 (3)	−0.5305 (3)	0.0781 (11)
H14C	0.1143	−0.5953	−0.5150	0.117*
H14A	0.0662	−0.4737	−0.4742	0.117*
H14B	0.1081	−0.4907	−0.5889	0.117*
O1	−0.1569 (2)	−0.61668 (18)	−0.38591 (17)	0.0618 (6)
H1	−0.233 (3)	−0.648 (3)	−0.3472 (19)	0.074*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0762 (5)	0.1058 (7)	0.0799 (7)	0.0203 (5)	−0.0073 (5)	0.0146 (6)
C11	0.072 (2)	0.0524 (19)	0.058 (2)	0.0033 (17)	0.0238 (19)	0.0008 (17)
C2	0.089 (3)	0.054 (2)	0.059 (2)	−0.0124 (19)	−0.002 (2)	0.0131 (19)
C4	0.064 (2)	0.065 (2)	0.083 (3)	−0.0066 (17)	0.016 (2)	0.000 (2)

C13	0.0515 (19)	0.0393 (16)	0.0471 (19)	0.0069 (13)	0.0008 (15)	−0.0042 (15)
N1	0.0543 (13)	0.0510 (14)	0.0477 (16)	−0.0051 (11)	0.0029 (14)	0.0016 (14)
C8	0.0473 (18)	0.0412 (17)	0.0452 (19)	0.0026 (12)	0.0044 (15)	−0.0075 (15)
C5	0.0581 (18)	0.0538 (19)	0.068 (2)	−0.0021 (15)	0.0058 (17)	0.0120 (18)
C1	0.0629 (18)	0.0511 (16)	0.0499 (19)	−0.0042 (15)	−0.0015 (18)	−0.0013 (18)
C3	0.087 (3)	0.064 (2)	0.067 (2)	−0.0186 (19)	0.022 (2)	0.002 (2)
C9	0.0564 (17)	0.0652 (18)	0.049 (2)	0.0009 (15)	−0.0027 (17)	−0.0051 (19)
C7	0.0468 (15)	0.0460 (16)	0.050 (2)	−0.0023 (14)	−0.0025 (16)	−0.0025 (17)
C12	0.0527 (17)	0.0432 (16)	0.057 (2)	0.0023 (14)	0.0098 (18)	−0.0034 (16)
C6	0.0539 (18)	0.0423 (16)	0.0523 (19)	−0.0094 (13)	0.0014 (16)	−0.0013 (17)
C10	0.079 (2)	0.071 (2)	0.042 (2)	0.0057 (18)	0.0028 (18)	−0.0004 (19)
C14	0.057 (2)	0.085 (2)	0.093 (3)	−0.0041 (17)	0.0114 (19)	0.004 (2)
O1	0.0516 (12)	0.0784 (16)	0.0554 (15)	−0.0011 (11)	−0.0025 (11)	0.0044 (12)

Geometric parameters (Å, °)

Cl1—C1	1.745 (3)	C8—C9	1.388 (4)
C11—C12	1.376 (4)	C8—C7	1.442 (4)
C11—C10	1.384 (4)	C5—C6	1.396 (4)
C11—H11	0.9300	C5—H5	0.9300
C2—C1	1.369 (4)	C1—C6	1.378 (4)
C2—C3	1.372 (4)	C3—H3	0.9300
C2—H2	0.9300	C9—C10	1.363 (4)
C4—C3	1.366 (4)	C9—H9	0.9300
C4—C5	1.379 (4)	C7—H7	0.9300
C4—H4	0.9300	C12—C14	1.503 (4)
C13—O1	1.351 (3)	C10—H10	0.9300
C13—C12	1.389 (4)	C14—H14C	0.9600
C13—C8	1.410 (4)	C14—H14A	0.9600
N1—C7	1.283 (3)	C14—H14B	0.9600
N1—C6	1.402 (3)	O1—H1	0.87 (3)
C12—C11—C10	122.2 (3)	C2—C3—H3	120.1
C12—C11—H11	118.9	C10—C9—C8	121.2 (3)
C10—C11—H11	118.9	C10—C9—H9	119.4
C1—C2—C3	119.7 (3)	C8—C9—H9	119.4
C1—C2—H2	120.1	N1—C7—C8	122.2 (3)
C3—C2—H2	120.1	N1—C7—H7	118.9
C3—C4—C5	120.5 (3)	C8—C7—H7	118.9
C3—C4—H4	119.8	C11—C12—C13	117.9 (3)
C5—C4—H4	119.8	C11—C12—C14	122.3 (3)
O1—C13—C12	117.5 (3)	C13—C12—C14	119.8 (3)
O1—C13—C8	121.4 (3)	C1—C6—C5	117.5 (3)
C12—C13—C8	121.1 (3)	C1—C6—N1	119.9 (3)
C7—N1—C6	121.1 (2)	C5—C6—N1	122.5 (3)
C9—C8—C13	118.3 (3)	C9—C10—C11	119.3 (3)
C9—C8—C7	120.0 (3)	C9—C10—H10	120.3
C13—C8—C7	121.7 (3)	C11—C10—H10	120.3
C4—C5—C6	120.4 (3)	C12—C14—H14C	109.5
C4—C5—H5	119.8	C12—C14—H14A	109.5

C6—C5—H5	119.8	H14C—C14—H14A	109.5
C2—C1—C6	122.0 (3)	C12—C14—H14B	109.5
C2—C1—Cl1	119.4 (3)	H14C—C14—H14B	109.5
C6—C1—Cl1	118.6 (2)	H14A—C14—H14B	109.5
C4—C3—C2	119.9 (3)	C13—O1—H1	108 (2)
C4—C3—H3	120.1		
O1—C13—C8—C9	−179.2 (2)	C10—C11—C12—C14	178.9 (3)
C12—C13—C8—C9	0.7 (4)	O1—C13—C12—C11	−179.7 (2)
O1—C13—C8—C7	2.5 (4)	C8—C13—C12—C11	0.4 (4)
C12—C13—C8—C7	−177.6 (2)	O1—C13—C12—C14	1.0 (4)
C3—C4—C5—C6	−0.6 (4)	C8—C13—C12—C14	−178.9 (3)
C3—C2—C1—C6	−1.1 (5)	C2—C1—C6—C5	1.1 (4)
C3—C2—C1—Cl1	−179.1 (3)	Cl1—C1—C6—C5	179.1 (2)
C5—C4—C3—C2	0.6 (5)	C2—C1—C6—N1	177.5 (3)
C1—C2—C3—C4	0.2 (5)	Cl1—C1—C6—N1	−4.5 (3)
C13—C8—C9—C10	−1.8 (4)	C4—C5—C6—C1	−0.2 (4)
C7—C8—C9—C10	176.5 (3)	C4—C5—C6—N1	−176.6 (3)
C6—N1—C7—C8	175.4 (2)	C7—N1—C6—C1	146.1 (3)
C9—C8—C7—N1	−176.7 (3)	C7—N1—C6—C5	−37.6 (4)
C13—C8—C7—N1	1.6 (4)	C8—C9—C10—C11	1.8 (5)
C10—C11—C12—C13	−0.4 (4)	C12—C11—C10—C9	−0.7 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.87 (1)	1.84 (2)	2.615 (3)	148 (3)

Fig. 1