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4-[(3-Chloro-2-methylphenyl)iminomethyl]phenol

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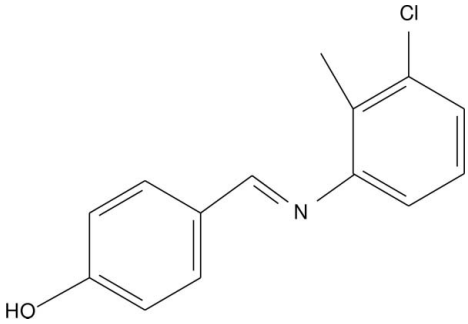
Key indicators: single-crystal X-ray study; T = 103 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.123; data-to-parameter ratio = 13.2.

In the title compound, $C_{14}H_{12}ClNO$, the dihedral angle between the aromatic rings is 39.84 (7)°. In th crystal, molecules are connected by O—H···N hydrogen bonds into chains parallel to [001]. In addition, a C—H···π contact occurs.

Related literature

For the bioactivity of the title compound, see: Corke *et al.* (1979); Gorrad & Manson (1989). For related structures, see: Jothi *et al.* (2012); Yaeghoobi *et al.* (2009).



Experimental

Crystal data

$C_{14}H_{12}ClNO$
M_r = 245.70
Orthorhombic, $P2_12_12_1$
a = 7.5271 (9) Å
b = 12.4095 (15) Å
c = 12.5800 (14) Å
V = 1175.1 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 103 K
0.26 × 0.20 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
6050 measured reflections
2042 independent reflections
1856 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.123
S = 1.07
2042 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

Cg is the centroid of the C11–C16 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N3^{i}	0.84	2.05	2.854 (3)	160
C17—H17C···Cg^{ii}	0.98	2.73	3.649 (2)	157

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

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KJ2211).

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supporting information

Acta Cryst. (2012). E**68**, o3191 [doi:10.1107/S1600536812043140]

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S1. Comment

The investigation of microbial degradation by hazardous compounds such as anilines containing a methyl and a chloro-substituent is of interest because of their lipophilic character and affinity to interact with DNA (Gorrad & Manson, 1989).

The *ORTEP* drawing of the title molecule is shown in Fig. 1. The 4-hydroxybenzylidene system is nearly planar and its geometry is similar to 4-chloro-2-[(*E*)-2-(4-methoxyphenyl)-ethyliminomethyl]phenol (Yaeghoobi *et al.*, 2009). The dihedral angle between the methylphenol and chloromethylphenylimino ring systems is 39.84 (7)°.

The molecules are connected by O—H···N interactions into chains along the [0 0 1] direction (Fig. 2). There is a weak contact of the type C—H···*π [1/2-x,-y,-1/2+z]* with a C···Cg distance of 3.649 (2) Å between the methyl group of the chloromethyl ring and the phenol ring.

S2. Experimental

Equimolar concentrations of 4-hydoxybenzaldehyde (0.003 mol) and 3-chloro-2-methylbenzenamine (0.003 mol) were refluxed for 5 h using methanol (25 ml) as solvent. The progress of the reaction was followed by TLC until the reaction was complete. The reaction product was cooled to 273 K. The precipitate was filtered and washed with diethyl ether. The residue was recrystallized from methanol. Brown single crystals were obtained.

S3. Refinement

In the absence of significant anomalous dispersion effects Friedel pairs have been merged. All the hydrogen atoms of the compound are fixed geometrically (O—H = 0.88 Å and C—H= 0.93–0.97 Å) and allowed to ride on their parent atoms.

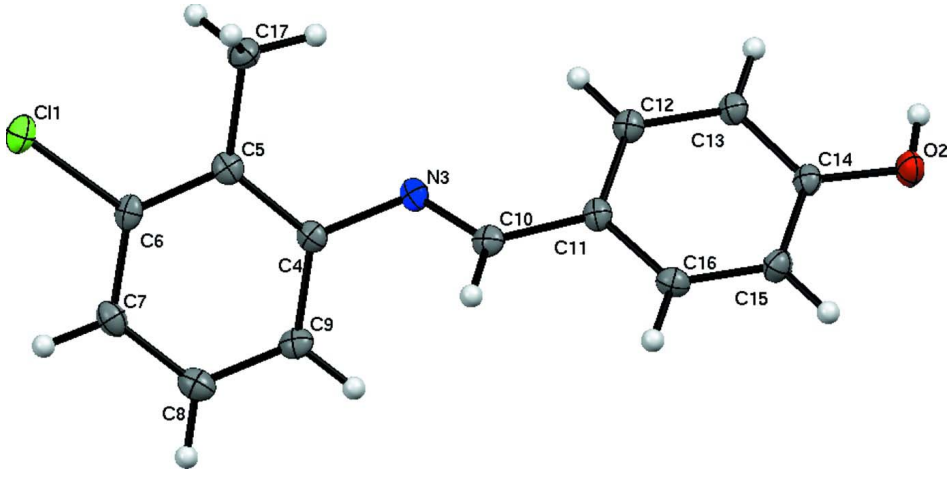

Figure 1

ORTEP diagram of the title compound with 50% probability ellipsoids.

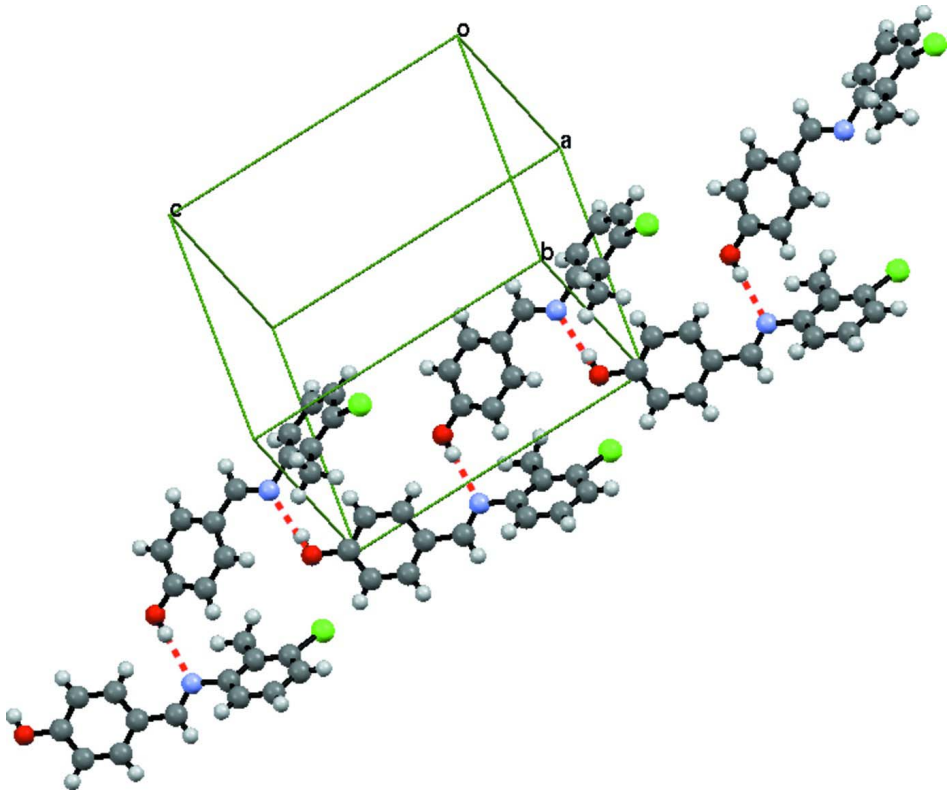

Figure 2

Packing diagram of the title compound, viewed along [1 - 1 0] direction. O—H···N hydrogen bonds are indicated by dashed lines.

4-[(3-Chloro-2-methylphenyl)iminomethyl]phenol

Crystal data

$C_{14}H_{12}ClNO$
$M_r = 245.70$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 7.5271$ (9) Å
$b = 12.4095$ (15) Å
$c = 12.5800$ (14) Å
$V = 1175.1$ (2) Å^3
$Z = 4$
$F(000) = 512$
$D_x = 1.389$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2042 reflections
$\theta = 2.3$–$30.6°$
$\mu = 0.31$ mm^{-1}
$T = 103$ K
Block, brown
0.26 × 0.20 × 0.18 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0839 pixels mm^{-1}
ω scans
6050 measured reflections
2042 independent reflections
1856 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 30.6°$, $\theta_{min} = 2.3°$
$h = -10 \rightarrow 7$
$k = -17 \rightarrow 16$
$l = -16 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.123$
$S = 1.07$
2042 reflections
155 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0838P)^2 + 0.0338P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.20725 (8)	0.07415 (5)	0.21487 (5)	0.0206 (2)
O2	−0.2400 (2)	0.06296 (14)	1.08991 (14)	0.0200 (5)
N3	−0.0186 (3)	0.11403 (16)	0.60025 (16)	0.0151 (5)
C4	0.0219 (3)	0.16256 (18)	0.50001 (19)	0.0142 (6)
C5	0.0934 (3)	0.09792 (18)	0.41844 (19)	0.0144 (6)
C6	0.1173 (3)	0.1473 (2)	0.31955 (19)	0.0147 (6)
C7	0.0749 (3)	0.2551 (2)	0.3006 (2)	0.0182 (7)
C8	0.0060 (3)	0.3171 (2)	0.3831 (2)	0.0192 (7)
C9	−0.0203 (3)	0.27089 (18)	0.4822 (2)	0.0165 (6)
C10	0.0205 (3)	0.16597 (19)	0.68499 (19)	0.0157 (6)
C11	−0.0336 (3)	0.13243 (19)	0.79125 (19)	0.0146 (6)
C12	−0.1136 (3)	0.03193 (19)	0.81002 (19)	0.0162 (6)
C13	−0.1794 (3)	0.00693 (19)	0.91011 (19)	0.0154 (6)
C14	−0.1689 (3)	0.08211 (19)	0.99228 (18)	0.0148 (6)
C15	−0.0820 (3)	0.18052 (19)	0.9758 (2)	0.0170 (6)
C16	−0.0153 (3)	0.20481 (19)	0.8757 (2)	0.0161 (6)
C17	0.1424 (3)	−0.01811 (19)	0.4369 (2)	0.0191 (7)
H2	−0.28810	0.00190	1.09040	0.0300*
H7	0.09280	0.28580	0.23230	0.0220*
H8	−0.02280	0.39070	0.37150	0.0230*
H9	−0.06730	0.31310	0.53850	0.0200*
H10	0.08860	0.23010	0.67830	0.0190*
H12	−0.12270	−0.01910	0.75400	0.0190*
H13	−0.23160	−0.06160	0.92270	0.0180*
H15	−0.06890	0.23030	1.03260	0.0200*

H16	0.04360	0.27160	0.86450	0.0190*
H17A	0.09600	−0.06240	0.37870	0.0290*
H17B	0.09100	−0.04250	0.50440	0.0290*
H17C	0.27200	−0.02500	0.43980	0.0290*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0193 (3)	0.0256 (3)	0.0169 (3)	−0.0005 (2)	0.0037 (2)	−0.0025 (2)
O2	0.0225 (9)	0.0216 (8)	0.0160 (8)	−0.0038 (7)	0.0057 (7)	−0.0002 (7)
N3	0.0108 (9)	0.0184 (9)	0.0160 (9)	−0.0002 (7)	0.0016 (8)	0.0019 (7)
C4	0.0096 (10)	0.0162 (10)	0.0168 (11)	−0.0014 (8)	0.0009 (9)	0.0013 (8)
C5	0.0083 (9)	0.0180 (10)	0.0170 (11)	−0.0006 (8)	−0.0017 (9)	0.0008 (8)
C6	0.0082 (9)	0.0213 (10)	0.0146 (10)	−0.0013 (8)	0.0015 (8)	−0.0017 (8)
C7	0.0150 (11)	0.0215 (11)	0.0180 (12)	−0.0024 (9)	0.0001 (9)	0.0043 (9)
C8	0.0147 (11)	0.0183 (11)	0.0246 (12)	−0.0002 (9)	−0.0011 (10)	0.0039 (9)
C9	0.0108 (10)	0.0173 (11)	0.0214 (12)	0.0014 (8)	0.0012 (9)	−0.0009 (9)
C10	0.0108 (10)	0.0171 (10)	0.0191 (11)	0.0005 (8)	0.0020 (9)	0.0000 (8)
C11	0.0104 (9)	0.0191 (10)	0.0144 (10)	0.0004 (8)	0.0002 (9)	0.0009 (9)
C12	0.0133 (10)	0.0189 (10)	0.0164 (11)	0.0002 (8)	−0.0002 (9)	−0.0003 (8)
C13	0.0121 (10)	0.0175 (10)	0.0167 (10)	−0.0003 (8)	0.0017 (9)	0.0002 (9)
C14	0.0121 (9)	0.0175 (10)	0.0148 (10)	0.0013 (8)	0.0016 (8)	0.0001 (8)
C15	0.0172 (11)	0.0178 (10)	0.0160 (11)	−0.0013 (9)	−0.0001 (10)	−0.0026 (8)
C16	0.0135 (11)	0.0151 (10)	0.0196 (11)	−0.0014 (8)	−0.0012 (9)	0.0008 (9)
C17	0.0185 (12)	0.0180 (11)	0.0207 (12)	0.0029 (9)	0.0033 (10)	0.0003 (9)

Geometric parameters (Å, º)

Cl1—C6	1.737 (2)	C12—C13	1.388 (3)
O2—C14	1.361 (3)	C13—C14	1.395 (3)
O2—H2	0.8400	C14—C15	1.401 (3)
N3—C4	1.430 (3)	C15—C16	1.389 (4)
N3—C10	1.280 (3)	C7—H7	0.9500
C4—C9	1.399 (3)	C8—H8	0.9500
C4—C5	1.409 (3)	C9—H9	0.9500
C5—C6	1.398 (3)	C10—H10	0.9500
C5—C17	1.504 (3)	C12—H12	0.9500
C6—C7	1.396 (3)	C13—H13	0.9500
C7—C8	1.392 (3)	C15—H15	0.9500
C8—C9	1.386 (4)	C16—H16	0.9500
C10—C11	1.458 (3)	C17—H17A	0.9800
C11—C16	1.398 (3)	C17—H17B	0.9800
C11—C12	1.405 (3)	C17—H17C	0.9800
C14—O2—H2	109.00	C11—C16—C15	120.9 (2)
C4—N3—C10	118.2 (2)	C6—C7—H7	120.00
N3—C4—C5	118.9 (2)	C8—C7—H7	120.00
C5—C4—C9	121.1 (2)	C7—C8—H8	120.00

N3—C4—C9	119.8 (2)	C9—C8—H8	120.00
C4—C5—C6	116.6 (2)	C4—C9—H9	120.00
C4—C5—C17	121.7 (2)	C8—C9—H9	120.00
C6—C5—C17	121.7 (2)	N3—C10—H10	118.00
Cl1—C6—C5	119.71 (18)	C11—C10—H10	118.00
Cl1—C6—C7	117.42 (18)	C11—C12—H12	120.00
C5—C6—C7	122.9 (2)	C13—C12—H12	120.00
C6—C7—C8	119.2 (2)	C12—C13—H13	120.00
C7—C8—C9	119.7 (2)	C14—C13—H13	120.00
C4—C9—C8	120.6 (2)	C14—C15—H15	120.00
N3—C10—C11	123.8 (2)	C16—C15—H15	120.00
C10—C11—C16	119.1 (2)	C11—C16—H16	120.00
C12—C11—C16	119.0 (2)	C15—C16—H16	119.00
C10—C11—C12	121.8 (2)	C5—C17—H17A	110.00
C11—C12—C13	120.3 (2)	C5—C17—H17B	109.00
C12—C13—C14	120.2 (2)	C5—C17—H17C	109.00
O2—C14—C13	122.0 (2)	H17A—C17—H17B	109.00
O2—C14—C15	118.0 (2)	H17A—C17—H17C	109.00
C13—C14—C15	120.0 (2)	H17B—C17—H17C	109.00
C14—C15—C16	119.5 (2)		

C10—N3—C4—C5	138.4 (2)	C6—C7—C8—C9	−0.4 (3)
C10—N3—C4—C9	−45.7 (3)	C7—C8—C9—C4	0.0 (3)
C4—N3—C10—C11	171.9 (2)	N3—C10—C11—C12	8.7 (4)
N3—C4—C5—C6	175.1 (2)	N3—C10—C11—C16	−167.4 (2)
N3—C4—C5—C17	−5.2 (3)	C10—C11—C12—C13	−173.6 (2)
C9—C4—C5—C6	−0.8 (3)	C16—C11—C12—C13	2.5 (3)
C9—C4—C5—C17	178.9 (2)	C10—C11—C16—C15	173.2 (2)
N3—C4—C9—C8	−175.3 (2)	C12—C11—C16—C15	−2.9 (3)
C5—C4—C9—C8	0.6 (3)	C11—C12—C13—C14	1.0 (3)
C4—C5—C6—Cl1	179.21 (17)	C12—C13—C14—O2	176.5 (2)
C4—C5—C6—C7	0.5 (3)	C12—C13—C14—C15	−4.0 (3)
C17—C5—C6—Cl1	−0.5 (3)	O2—C14—C15—C16	−177.0 (2)
C17—C5—C6—C7	−179.2 (2)	C13—C14—C15—C16	3.5 (3)
Cl1—C6—C7—C8	−178.66 (18)	C14—C15—C16—C11	0.0 (3)
C5—C6—C7—C8	0.1 (3)		

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C11–C16 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N3^{i}	0.84	2.05	2.854 (3)	160
C12—H12···O2^{ii}	0.95	2.37	3.204 (3)	146
C17—H17*B*···N3	0.98	2.43	2.895 (3)	108
C17—H17*C*···*Cg*^{iii}	0.98	2.73	3.649 (2)	157

Symmetry codes: (i) −*x*−1/2, −*y*, *z*+1/2; (ii) −*x*−1/2, −*y*, *z*−1/2; (iii) −*x*+1/2, −*y*, *z*−1/2.