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4-Chloro-2-[(*E*)-2-(4-methoxyphenyl)-ethyliminomethyl]phenol

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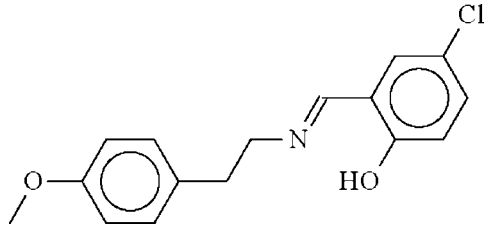
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.099; data-to-parameter ratio = 16.3.

In the title Schiff base, $C_{16}H_{16}ClNO_2$, the 2-(4-methoxyphenyl)ethyl ($CH_3OC_6H_4CH_2CH_2$–; r.m.s. deviation = 0.10 Å) and 4-chloro-2-(iminomethyl)phenol (N=CHC_6H_3ClOH; r.m.s. deviation = 0.01 Å) portions are both essentially planar, the two parts being inclined at an angle of 61.8 (1)°. The hydroxy group forms a hydrogen bond to the imino N atom.

Related literature

The crystal structures of several Schiff bases derived by condensing aryl-2-ethylamines and substituted salicylaldehydes have been reported; see: Chatziefthimiou *et al.* (2006); Chohan *et al.* (2008); Coombs *et al.* (2005); Li *et al.* (2006); Räisänen *et al.* (2007).



Experimental

Crystal data

$C_{16}H_{16}ClNO_2$
M_r = 289.75
Triclinic, $P\overline{1}$
a = 5.7610 (2) Å
b = 7.7115 (3) Å
c = 15.7814 (5) Å
α = 82.420 (2)°
β = 89.320 (2)°
γ = 85.313 (2)°
V = 692.65 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 100 K
0.25 × 0.25 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.934, T_{max} = 0.992
5284 measured reflections
3036 independent reflections
2235 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.099
S = 1.03
3036 reflections
186 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.85 (1)	1.79 (2)	2.567 (2)	152 (3)

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2612).

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supporting information

Acta Cryst. (2009). E**65**, o1070 [doi:10.1107/S1600536809013348]

4-Chloro-2-[(*E*)-2-(4-methoxyphenyl)ethyliminomethyl]phenol

Marzieh Yaeghoobi, Noorsaadah Abdul Rahman and Seik Weng Ng

S1. Experimental

2-(4-Methoxyphenyl)ethylamine (0.30 g, 2 mmol) and 5-chlorosalicylaldehyde (0.31 g, 2 mmol) were heated in ethanol (20 ml) for 1 h. The solution was set aside for the growth of crystals.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with *U*(H) fixed at 1.2–1.5*U*(C).

The hydroxy H-atom was located in a difference Fourier map, and was refined with a distance restraint of O–H 0.84±0.01 Å; its temperature factor was refined.

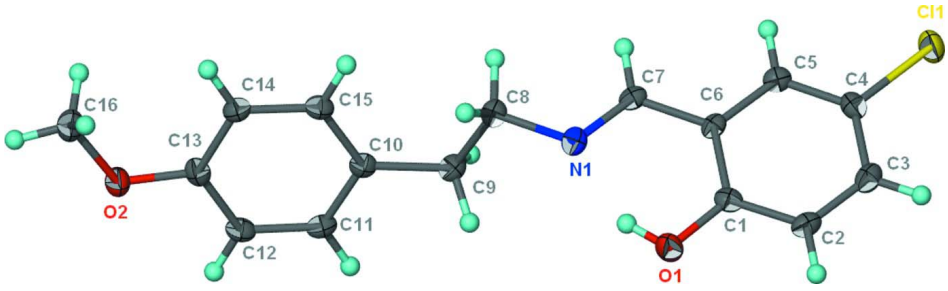

Figure 1

Thermal ellipsoid plot of $C_{16}H_{16}ClNO_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-Chloro-2-[(*E*)-2-(4-methoxyphenyl)ethyliminomethyl]phenol

Crystal data

$C_{16}H_{16}ClNO_2$
$M_r = 289.75$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.7610\ (2)$ Å
$b = 7.7115\ (3)$ Å
$c = 15.7814\ (5)$ Å
$\alpha = 82.420\ (2)°$
$\beta = 89.320\ (2)°$
$\gamma = 85.313\ (2)°$
$V = 692.65\ (4)$ Å^3
$Z = 2$
$F(000) = 304$
$D_x = 1.389$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1628 reflections
$\theta = 2.7–28.2°$
$\mu = 0.28$ mm^{-1}
$T = 100$ K
Plate, yellow
0.25 × 0.25 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.934, T_{max} = 0.992
5284 measured reflections
3036 independent reflections
2235 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.5°, θ_{min} = 2.6°
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 9$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.099
S = 1.03
3036 reflections
186 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.033P)^2 + 0.4582P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.72711 (10)	0.19401 (7)	0.02737 (3)	0.02303 (15)
O1	0.4122 (3)	0.0304 (2)	0.38188 (9)	0.0209 (3)
H1	0.509 (4)	0.068 (4)	0.4137 (15)	0.042 (8)*
O2	0.9991 (2)	0.43513 (19)	0.88357 (8)	0.0184 (3)
N1	0.7683 (3)	0.1729 (2)	0.42911 (10)	0.0157 (4)
C1	0.4895 (3)	0.0673 (3)	0.30093 (12)	0.0147 (4)
C2	0.3616 (3)	0.0202 (3)	0.23431 (13)	0.0168 (4)
H2	0.2243	−0.0389	0.2465	0.020*
C3	0.4334 (4)	0.0592 (3)	0.15057 (13)	0.0177 (4)
H3	0.3449	0.0282	0.1053	0.021*
C4	0.6357 (4)	0.1440 (3)	0.13294 (12)	0.0161 (4)
C5	0.7667 (3)	0.1895 (3)	0.19782 (12)	0.0150 (4)
H5	0.9056	0.2460	0.1847	0.018*
C6	0.6960 (3)	0.1530 (2)	0.28272 (12)	0.0130 (4)
C7	0.8351 (3)	0.2023 (3)	0.35138 (12)	0.0139 (4)
H7	0.9757	0.2564	0.3381	0.017*
C8	0.9076 (3)	0.2214 (3)	0.49754 (12)	0.0157 (4)
H8A	1.0524	0.2691	0.4737	0.019*
H8B	0.9509	0.1165	0.5393	0.019*
C9	0.7660 (3)	0.3591 (3)	0.54177 (12)	0.0159 (4)
H9A	0.7698	0.4739	0.5056	0.019*
H9B	0.6019	0.3293	0.5451	0.019*
C10	0.8459 (3)	0.3790 (3)	0.63111 (12)	0.0142 (4)
C11	0.6936 (3)	0.4703 (3)	0.68291 (13)	0.0158 (4)

H11	0.5482	0.5219	0.6603	0.019*
C12	0.7501 (4)	0.4870 (3)	0.76572 (13)	0.0163 (4)
H12	0.6443	0.5498	0.7995	0.020*
C13	0.9625 (4)	0.4120 (3)	0.80025 (12)	0.0159 (4)
C14	1.1189 (4)	0.3236 (3)	0.75010 (12)	0.0152 (4)
H14	1.2652	0.2739	0.7726	0.018*
C15	1.0580 (3)	0.3086 (3)	0.66572 (13)	0.0156 (4)
H15	1.1654	0.2486	0.6314	0.019*
C16	1.2113 (4)	0.3563 (3)	0.92316 (13)	0.0212 (5)
H16A	1.2147	0.3805	0.9825	0.032*
H16B	1.3442	0.4054	0.8920	0.032*
H16C	1.2202	0.2292	0.9220	0.032*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0271 (3)	0.0286 (3)	0.0145 (2)	−0.0072 (2)	0.0018 (2)	−0.0036 (2)
O1	0.0214 (8)	0.0262 (9)	0.0161 (7)	−0.0088 (7)	0.0029 (6)	−0.0026 (6)
O2	0.0195 (8)	0.0215 (8)	0.0141 (7)	−0.0005 (6)	−0.0014 (6)	−0.0023 (6)
N1	0.0174 (9)	0.0134 (9)	0.0164 (8)	−0.0008 (7)	−0.0022 (7)	−0.0024 (7)
C1	0.0144 (10)	0.0119 (10)	0.0172 (10)	0.0019 (8)	0.0020 (8)	−0.0011 (8)
C2	0.0130 (10)	0.0151 (10)	0.0226 (11)	−0.0015 (8)	−0.0012 (8)	−0.0033 (8)
C3	0.0171 (10)	0.0153 (10)	0.0211 (10)	−0.0005 (8)	−0.0045 (8)	−0.0046 (8)
C4	0.0181 (11)	0.0159 (10)	0.0139 (9)	0.0008 (8)	0.0014 (8)	−0.0016 (8)
C5	0.0144 (10)	0.0118 (10)	0.0185 (10)	−0.0008 (8)	−0.0001 (8)	−0.0011 (8)
C6	0.0121 (10)	0.0108 (10)	0.0157 (9)	0.0014 (8)	−0.0030 (8)	−0.0014 (8)
C7	0.0116 (10)	0.0109 (10)	0.0190 (10)	−0.0001 (8)	−0.0017 (8)	−0.0011 (8)
C8	0.0167 (10)	0.0141 (10)	0.0162 (10)	−0.0007 (8)	−0.0019 (8)	−0.0020 (8)
C9	0.0158 (10)	0.0136 (10)	0.0182 (10)	−0.0010 (8)	−0.0019 (8)	−0.0022 (8)
C10	0.0149 (10)	0.0112 (10)	0.0167 (10)	−0.0041 (8)	0.0014 (8)	−0.0010 (8)
C11	0.0119 (10)	0.0133 (10)	0.0217 (10)	−0.0006 (8)	−0.0001 (8)	−0.0014 (8)
C12	0.0148 (10)	0.0141 (10)	0.0199 (10)	0.0001 (8)	0.0033 (8)	−0.0030 (8)
C13	0.0203 (11)	0.0137 (10)	0.0138 (9)	−0.0050 (8)	0.0018 (8)	−0.0008 (8)
C14	0.0128 (10)	0.0147 (10)	0.0179 (10)	−0.0006 (8)	−0.0005 (8)	−0.0013 (8)
C15	0.0140 (10)	0.0143 (10)	0.0184 (10)	−0.0003 (8)	0.0023 (8)	−0.0027 (8)
C16	0.0228 (11)	0.0236 (12)	0.0172 (10)	−0.0034 (9)	−0.0027 (9)	−0.0022 (9)

Geometric parameters (Å, º)

Cl1—C4	1.745 (2)	C8—H8A	0.9900
O1—C1	1.350 (2)	C8—H8B	0.9900
O1—H1	0.849 (10)	C9—C10	1.519 (3)
O2—C13	1.371 (2)	C9—H9A	0.9900
O2—C16	1.432 (3)	C9—H9B	0.9900
N1—C7	1.278 (2)	C10—C15	1.384 (3)
N1—C8	1.458 (2)	C10—C11	1.403 (3)
C1—C2	1.394 (3)	C11—C12	1.375 (3)
C1—C6	1.415 (3)	C11—H11	0.9500

C2—C3	1.382 (3)	C12—C13	1.395 (3)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.390 (3)	C13—C14	1.388 (3)
C3—H3	0.9500	C14—C15	1.403 (3)
C4—C5	1.378 (3)	C14—H14	0.9500
C5—C6	1.395 (3)	C15—H15	0.9500
C5—H5	0.9500	C16—H16A	0.9800
C6—C7	1.463 (3)	C16—H16B	0.9800
C7—H7	0.9500	C16—H16C	0.9800
C8—C9	1.523 (3)		

C1—O1—H1	106.3 (19)	C10—C9—C8	115.68 (17)
C13—O2—C16	117.54 (16)	C10—C9—H9A	108.4
C7—N1—C8	120.28 (17)	C8—C9—H9A	108.4
O1—C1—C2	118.87 (17)	C10—C9—H9B	108.4
O1—C1—C6	121.37 (17)	C8—C9—H9B	108.4
C2—C1—C6	119.77 (17)	H9A—C9—H9B	107.4
C3—C2—C1	120.33 (18)	C15—C10—C11	117.62 (18)
C3—C2—H2	119.8	C15—C10—C9	124.08 (18)
C1—C2—H2	119.8	C11—C10—C9	118.28 (18)
C2—C3—C4	119.71 (18)	C12—C11—C10	121.49 (19)
C2—C3—H3	120.1	C12—C11—H11	119.3
C4—C3—H3	120.1	C10—C11—H11	119.3
C5—C4—C3	120.97 (18)	C11—C12—C13	120.15 (18)
C5—C4—Cl1	119.05 (15)	C11—C12—H12	119.9
C3—C4—Cl1	119.98 (15)	C13—C12—H12	119.9
C4—C5—C6	120.20 (18)	O2—C13—C14	125.16 (19)
C4—C5—H5	119.9	O2—C13—C12	115.10 (17)
C6—C5—H5	119.9	C14—C13—C12	119.73 (18)
C5—C6—C1	119.01 (17)	C13—C14—C15	119.15 (19)
C5—C6—C7	120.01 (17)	C13—C14—H14	120.4
C1—C6—C7	120.98 (17)	C15—C14—H14	120.4
N1—C7—C6	120.31 (17)	C10—C15—C14	121.83 (18)
N1—C7—H7	119.8	C10—C15—H15	119.1
C6—C7—H7	119.8	C14—C15—H15	119.1
N1—C8—C9	108.99 (16)	O2—C16—H16A	109.5
N1—C8—H8A	109.9	O2—C16—H16B	109.5
C9—C8—H8A	109.9	H16A—C16—H16B	109.5
N1—C8—H8B	109.9	O2—C16—H16C	109.5
C9—C8—H8B	109.9	H16A—C16—H16C	109.5
H8A—C8—H8B	108.3	H16B—C16—H16C	109.5

O1—C1—C2—C3	178.70 (19)	C7—N1—C8—C9	117.2 (2)
C6—C1—C2—C3	−1.0 (3)	N1—C8—C9—C10	159.86 (16)
C1—C2—C3—C4	0.7 (3)	C8—C9—C10—C15	13.5 (3)
C2—C3—C4—C5	0.2 (3)	C8—C9—C10—C11	−164.78 (17)
C2—C3—C4—Cl1	−179.87 (16)	C15—C10—C11—C12	−1.2 (3)
C3—C4—C5—C6	−0.9 (3)	C9—C10—C11—C12	177.17 (18)

Cl1—C4—C5—C6	179.22 (16)	C10—C11—C12—C13	−0.2 (3)
C4—C5—C6—C1	0.6 (3)	C16—O2—C13—C14	−2.5 (3)
C4—C5—C6—C7	−179.72 (19)	C16—O2—C13—C12	178.17 (17)
O1—C1—C6—C5	−179.34 (18)	C11—C12—C13—O2	−179.27 (18)
C2—C1—C6—C5	0.3 (3)	C11—C12—C13—C14	1.4 (3)
O1—C1—C6—C7	1.0 (3)	O2—C13—C14—C15	179.56 (18)
C2—C1—C6—C7	−179.37 (18)	C12—C13—C14—C15	−1.2 (3)
C8—N1—C7—C6	179.71 (17)	C11—C10—C15—C14	1.5 (3)
C5—C6—C7—N1	178.33 (19)	C9—C10—C15—C14	−176.86 (18)
C1—C6—C7—N1	−2.0 (3)	C13—C14—C15—C10	−0.3 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.85 (1)	1.79 (2)	2.567 (2)	152 (3)