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2-(Benzyliminomethyl)-6-methoxyphenol

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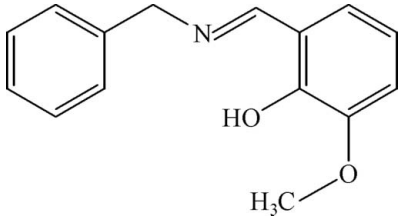
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.058; wR factor = 0.202; data-to-parameter ratio = 17.9.

In the title Schiff base compound, $C_{15}H_{15}NO_2$, the C=N and C—N bond lengths are 1.277 (4) and 1.453 (5) Å, respectively, while the C—O bond length of the hydroxyl group is 1.334 (3) Å. The molecule exhibits an intramolecular O—H···N hydrogen bond with an O···N distance of 2.548 (3) Å.

Related literature

For related literature, see: Bhadbhade & Srinivas (1993); Bunce *et al.* (1998); Garnovskii *et al.* (1993); Huang *et al.* (2002).



Experimental

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Monoclinic, $P2_1/c$
a = 8.9236 (2) Å
b = 5.7681 (1) Å
c = 23.8006 (2) Å
β = 92.432 (2)°
V = 1223.97 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
0.26 × 0.24 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.978, T_{max} = 0.990
8962 measured reflections
2958 independent reflections
1876 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.202
S = 1.00
2958 reflections
165 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···N1	0.82	1.81	2.548 (3)	150

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BI2232).

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supplementary materials

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2-(Benzyliminomethyl)-6-methoxyphenol

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Comment

Schiff bases have been utilized as ligands for a long time due to their straightforward synthesis and versatility in metal complexes. They therefore play an important role in the development of coordination chemistry as well as inorganic biochemistry, catalysis, optical materials and so on (Garnovskii *et al.*, 1993; Huang *et al.*, 2002). Considerable attention has been focused on the syntheses and structures of copper(II) and nickel(II) complexes. The nickel complexes with multidentate Schiff-base ligands have aroused particular interest because this metal can exhibit several oxidation states and may provide the basis for models of active sites of biological systems. The main attention with optically active Schiff-base complexes is concentrated on their catalytic abilities in stereo-selective synthesis (Bhadbhade & Srinivas, 1993; Bunce *et al.*, 1998). As part of our research aiming to understand the molecular properties of chiral Schiff-base complexes, we describe here the synthesis and crystal structure of the title Schiff-base ligand (Figure 1).

Experimental

A mixture of benzylamine (5.00 mmol) and *o*-vanillin (5.00 mmol) in methanol (40 ml) was refluxed with stirring for one hour to give an orange precipitate which was filtered and washed with methanol to give the title compound in 86% yield. Elemental analysis calculated: C 74.69, H 6.22, N 5.81%; found: C 74.66, H 6.12, N 5.79%.

Refinement

H atoms were positioned geometrically with O—H = 0.82 Å and C—H = 0.93 or 0.96 Å, then constrained to ride on their parent atoms with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H, and 1.2 for all other H atoms.

Figures

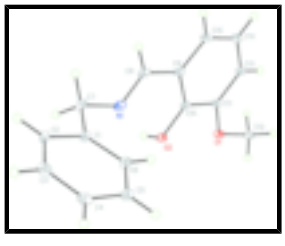

Fig. 1. The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms.

2-(Benzyliminomethyl)-6-methoxyphenol

Crystal data

$C_{15}H_{15}NO_2$	F_{000} = 512
M_r = 241.28	D_x = 1.309 Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 2958 reflections
$a = 8.9236$ (2) Å	$\theta = 2.3$–28.1°
$b = 5.7681$ (1) Å	$\mu = 0.09$ mm^{-1}
$c = 23.8006$ (2) Å	$T = 293$ (2) K
$\beta = 92.432$ (2)°	Block, colourless
$V = 1223.97$ (4) Å^3	0.26 × 0.24 × 0.12 mm
$Z = 4$	

Data collection

Bruker APEXII CCD diffractometer	2958 independent reflections
Radiation source: fine-focus sealed tube	1876 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 293(2)$ K	$\theta_{max} = 28.1^\circ$
φ and ω scans	$\theta_{min} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$h = -10 \rightarrow 11$
$T_{min} = 0.978$, $T_{max} = 0.990$	$k = -7 \rightarrow 7$
8962 measured reflections	$l = -31 \rightarrow 31$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H-atom parameters constrained
$wR(F^2) = 0.202$	$w = 1/[\sigma^2(F_o^2) + (0.1284P)^2 + 0.1359P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.003$
2958 reflections	$\Delta\rho_{max} = 0.45$ e Å^{-3}
165 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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}
C1	0.2240 (3)	0.5473 (5)	−0.01082 (11)	0.0597 (7)
C2	0.2308 (3)	0.3654 (5)	−0.04596 (12)	0.0640 (7)
H11	0.2868	0.2332	−0.0373	0.077*
C3	0.1488 (4)	0.3901 (8)	−0.09541 (16)	0.0889 (11)
H18	0.1501	0.2699	−0.1214	0.107*
C4	0.0667 (4)	0.5786 (8)	−0.10837 (15)	0.0832 (10)
H15	0.0116	0.5850	−0.1424	0.100*
C5	0.0631 (4)	0.7614 (7)	−0.07204 (15)	0.0821 (10)
H17	0.0074	0.8934	−0.0811	0.098*
C6	0.1428 (4)	0.7460 (6)	−0.02230 (13)	0.0705 (8)
H14	0.1425	0.8672	0.0035	0.085*
C7	0.3131 (4)	0.5078 (7)	0.04205 (13)	0.0771 (9)
H12A	0.2776	0.3682	0.0599	0.093*
H12B	0.4172	0.4837	0.0334	0.093*
C8	0.4167 (3)	0.8313 (7)	0.09167 (11)	0.0698 (9)
H7	0.5043	0.8025	0.0730	0.084*
C9	0.4159 (3)	1.0214 (6)	0.13121 (11)	0.0627 (8)
C10	0.2909 (3)	1.0611 (5)	0.16243 (10)	0.0561 (7)
C11	0.2914 (3)	1.2476 (5)	0.20011 (11)	0.0597 (7)
C12	0.1536 (4)	1.4678 (7)	0.26392 (15)	0.0782 (9)
H13A	0.2306	1.4617	0.2933	0.117*
H13B	0.0570	1.4676	0.2802	0.117*
H13C	0.1648	1.6068	0.2423	0.117*
C13	0.4141 (3)	1.3927 (6)	0.20707 (13)	0.0690 (8)
H9	0.4130	1.5144	0.2327	0.083*
C14	0.5364 (3)	1.3557 (7)	0.17609 (15)	0.0773 (9)
H16	0.6190	1.4535	0.1801	0.093*
C15	0.5382 (3)	1.1745 (7)	0.13892 (13)	0.0753 (10)
H8	0.6228	1.1517	0.1181	0.090*
N1	0.3035 (3)	0.7008 (5)	0.08094 (9)	0.0697 (7)
O1	0.1661 (2)	1.2709 (4)	0.22824 (9)	0.0730 (7)
O2	0.1710 (2)	0.9237 (4)	0.15680 (8)	0.0670 (6)
H2	0.1852	0.8256	0.1327	0.101*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0579 (15)	0.0649 (17)	0.0569 (14)	0.0073 (12)	0.0109 (11)	0.0053 (12)
C2	0.0709 (17)	0.0586 (16)	0.0630 (15)	0.0114 (13)	0.0089 (13)	−0.0047 (13)
C3	0.088 (2)	0.101 (3)	0.078 (2)	−0.012 (2)	0.0095 (18)	−0.023 (2)
C4	0.067 (2)	0.116 (3)	0.0658 (18)	−0.012 (2)	−0.0051 (14)	0.0036 (19)
C5	0.074 (2)	0.093 (3)	0.078 (2)	0.0119 (17)	−0.0122 (16)	0.0131 (18)
C6	0.0740 (18)	0.0723 (19)	0.0648 (16)	0.0136 (15)	−0.0014 (14)	0.0005 (15)
C7	0.082 (2)	0.088 (2)	0.0613 (17)	0.0314 (18)	0.0042 (14)	0.0068 (16)

C8	0.0531 (15)	0.106 (2)	0.0503 (13)	0.0250 (16)	0.0068 (11)	0.0195 (15)
C9	0.0455 (13)	0.095 (2)	0.0476 (13)	0.0132 (13)	0.0032 (10)	0.0198 (13)
C10	0.0406 (12)	0.0800 (18)	0.0477 (12)	0.0038 (11)	0.0003 (9)	0.0160 (12)
C11	0.0477 (13)	0.0786 (19)	0.0530 (13)	0.0035 (12)	0.0028 (10)	0.0137 (13)
C12	0.0698 (18)	0.100 (3)	0.0659 (17)	0.0036 (17)	0.0089 (14)	−0.0046 (17)
C13	0.0538 (15)	0.085 (2)	0.0675 (16)	−0.0037 (14)	−0.0020 (12)	0.0145 (15)
C14	0.0515 (15)	0.102 (3)	0.0781 (19)	−0.0111 (16)	0.0025 (13)	0.0179 (19)
C15	0.0411 (13)	0.119 (3)	0.0662 (17)	0.0057 (15)	0.0086 (11)	0.0276 (19)
N1	0.0616 (14)	0.0969 (19)	0.0508 (12)	0.0196 (13)	0.0033 (10)	0.0071 (12)
O1	0.0525 (11)	0.0963 (17)	0.0711 (12)	−0.0048 (10)	0.0131 (9)	−0.0105 (11)
O2	0.0489 (10)	0.0910 (16)	0.0617 (11)	−0.0020 (9)	0.0083 (8)	−0.0016 (10)

Geometric parameters (Å, °)

C1—C2	1.345 (4)	C8—H7	0.930
C1—C6	1.378 (4)	C9—C10	1.386 (4)
C1—C7	1.477 (4)	C9—C15	1.409 (5)
C2—C3	1.367 (5)	C10—O2	1.334 (3)
C2—H11	0.930	C10—C11	1.401 (4)
C3—C4	1.340 (6)	C11—O1	1.334 (3)
C3—H18	0.930	C11—C13	1.383 (4)
C4—C5	1.365 (5)	C12—O1	1.425 (4)
C4—H15	0.930	C12—H13A	0.960
C5—C6	1.357 (5)	C12—H13B	0.960
C5—H17	0.930	C12—H13C	0.960
C6—H14	0.930	C13—C14	1.360 (4)
C7—N1	1.453 (5)	C13—H9	0.930
C7—H12A	0.970	C14—C15	1.370 (5)
C7—H12B	0.970	C14—H16	0.930
C8—N1	1.277 (4)	C15—H8	0.930
C8—C9	1.445 (5)	O2—H2	0.820
C2—C1—C6	124.3 (3)	C10—C9—C15	117.6 (3)
C2—C1—C7	111.9 (3)	C10—C9—C8	120.0 (3)
C6—C1—C7	123.8 (3)	C15—C9—C8	122.4 (3)
C1—C2—C3	114.7 (3)	O2—C10—C9	120.6 (3)
C1—C2—H11	122.7	O2—C10—C11	120.1 (2)
C3—C2—H11	122.7	C9—C10—C11	119.3 (3)
C4—C3—C2	123.4 (3)	O1—C11—C13	123.8 (3)
C4—C3—H18	118.3	O1—C11—C10	114.7 (2)
C2—C3—H18	118.3	C13—C11—C10	121.5 (2)
C3—C4—C5	120.5 (3)	O1—C12—H13A	109.5
C3—C4—H15	119.7	O1—C12—H13B	109.5
C5—C4—H15	119.7	H13A—C12—H13B	109.5
C6—C5—C4	118.5 (3)	O1—C12—H13C	109.5
C6—C5—H17	120.8	H13A—C12—H13C	109.5
C4—C5—H17	120.8	H13B—C12—H13C	109.5
C5—C6—C1	118.6 (3)	C14—C13—C11	119.3 (3)
C5—C6—H14	120.7	C14—C13—H9	120.3
C1—C6—H14	120.7	C11—C13—H9	120.3

N1—C7—C1	112.4 (3)	C13—C14—C15	120.1 (3)
N1—C7—H12A	109.1	C13—C14—H16	120.0
C1—C7—H12A	109.1	C15—C14—H16	120.0
N1—C7—H12B	109.1	C14—C15—C9	122.2 (3)
C1—C7—H12B	109.1	C14—C15—H8	118.9
H12A—C7—H12B	107.9	C9—C15—H8	118.9
N1—C8—C9	123.5 (3)	C8—N1—C7	120.8 (3)
N1—C8—H7	118.2	C11—O1—C12	117.9 (2)
C9—C8—H7	118.2	C10—O2—H2	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···N1	0.82	1.81	2.548 (3)	150

Fig. 1