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2-[(4-Methoxybenzyl)iminomethyl]-phenol

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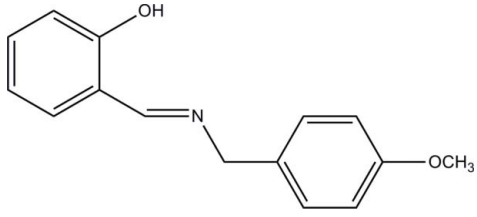
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.051; wR factor = 0.162; data-to-parameter ratio = 9.6.

In the title Schiff base compound, $C_{15}H_{15}NO_2$, prepared from 4-methoxybenzylamine and salicylaldehyde, an intramolecular O—H···N hydrogen bonds influences the molecular conformation; the two aromatic rings form a dihedral angle of 73.5 (1)°. In the crystal, weak intermolecular C—H···O interactions link the molecules into chains propagating in [010].

Related literature

For background to Schiff base ligands and their biological activity, see: Adsule *et al.* (2006); Karthikeyan *et al.* (2006). For related structures, see: Phurat *et al.* (2010); Tariq *et al.* (2010); Khalaji & Simpson (2009). For the graph-set analysis of hydrogen-bond patterns, see: Bernstein *et al.* (1995). For details of the synthesis, see: Phurat *et al.* (2010); Kannappan *et al.* (2005).



Experimental

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Orthorhombic, $P2_12_12_1$
a = 5.7190 (8) Å
b = 12.7229 (19) Å
c = 17.936 (3) Å
V = 1305.0 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.3 × 0.18 × 0.04 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
5776 measured reflections
1573 independent reflections
1177 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.162
S = 1.13
1573 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.82	1.85	2.574 (3)	146
C11—H11···O1^{i}	0.93	2.54	3.464 (4)	175

Symmetry code: (i) $-x+3, y+\frac{1}{2}, -z+\frac{3}{2}$.

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: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2800).

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supporting information

Acta Cryst. (2010). E**66**, o3298 [https://doi.org/10.1107/S1600536810048282]

2-[(4-Methoxybenzyl)iminomethyl]phenol

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S1. Comment

Schiff base complexes have gained importance from physiological and pharmacological activities point of view (Adsule *et al.*, 2006; Karthikeyan *et al.*, 2006). As a part of our research focused on the area of transition metal complex-based anticancer agents, the title compound (I) has been prepared as a ligand by Schiff base reaction between 4-methoxybenzylamine and salicylaldehyde.

The molecule of (I) (Fig. 1) adopts a *V*-shape structure. The dihedral angle between the methoxybenzene ring and 2-methyliminophenol moiety is 73.5 (1)°. The 2-methyliminophenol (C1 to C7, N1 and O1) moiety is nearly planar (r.m.s. deviation = 0.021 Å). The methoxybenzene and 2-methyliminophenol groups are located on the opposite side of the C=N bond, showing an *E* configuration. The bond lengths and angles in (I) are normal and comparable with those observed in the related compounds (Phurat *et al.*, 2010; Tariq *et al.*, 2010; Khalaji & Simpson, 2009). Intramolecular O—H···N hydrogen bond (Table 1) generates a S(6) ring (Bernstein *et al.*, 1995).

In the crystal structure, weak intermolecular C—H···O interactions (Table 1) link the molecules into chains propagated in direction [010].

S2. Experimental

The title compound was prepared according to the method reported in the literature (Kannappan *et al.*, 2005; Phurat *et al.*, 2010). 4-Methoxybenzylamine (2.50 ml.2.63 g, 0.02 mol) was added to a stirred ethanol solution of salicylaldehyde (2.50 ml, 2.86 g, 0.02 mol). The reaction mixture was stirred at reflux for 2 h and then the mixture was allowed to stand at room temperature for 1 week to give yellow cystals suitable for X-ray diffraction analysis.

S3. Refinement

H-atoms were geometrically positioned (C—H 0.93-0.97 Å, O—H 0.82 Å) and refined using a riding model, with U_{iso}= 1.2-1.5 U_{eq} of the parent atom. The absolute structure could not be determined and therefore 1,086 Friedel opposites were merged.

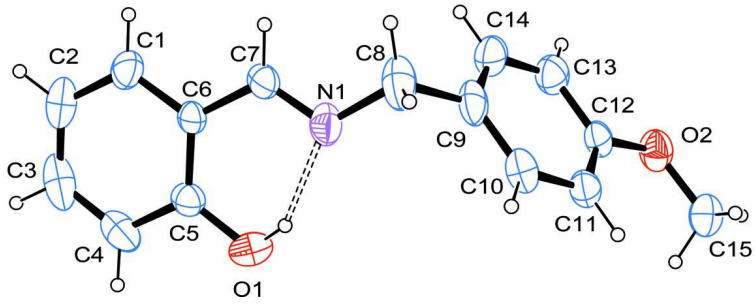

Figure 1

The molecular structure of (I) with displacement ellipsoids for the non-hydrogen atoms drawn at the 30% probability level. Hydrogen bond is shown as a dashed line.

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$V = 1305.0\ (3)$ Å^3
$Z = 4$
$F(000) = 512$
$D_x = 1.228$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Needle, yellow
0.3 × 0.18 × 0.04 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: Mo Kα
Graphite monochromator
φ and ω scans
5776 measured reflections
1573 independent reflections
1177 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.0°$
$h = -7\rightarrow7$
$k = -15\rightarrow14$
$l = -20\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.162$
$S = 1.13$
1573 reflections
164 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.7854 (7)	0.1595 (3)	0.54878 (17)	0.0795 (9)
H1	0.642	0.183	0.5308	0.095*
C2	0.8661 (10)	0.0614 (3)	0.5283 (2)	0.1029 (14)
H2	0.7787	0.0191	0.4965	0.123*
C3	1.0749 (9)	0.0274 (3)	0.5552 (3)	0.1095 (15)
H3	1.1283	−0.039	0.5417	0.131*
C4	1.2087 (7)	0.0879 (3)	0.6015 (2)	0.0909 (11)
H4	1.3499	0.0627	0.6199	0.109*
C5	1.1300 (5)	0.1875 (2)	0.62042 (17)	0.0668 (8)
C6	0.9144 (5)	0.2235 (2)	0.59563 (14)	0.0570 (6)
C7	0.8246 (5)	0.3261 (2)	0.61737 (18)	0.0675 (7)
H7	0.6806	0.3482	0.599	0.081*
C8	0.8369 (7)	0.4881 (3)	0.6807 (3)	0.1079 (14)
H8A	0.7999	0.4889	0.7335	0.129*
H8B	0.6929	0.4989	0.6532	0.129*
C9	1.0065 (6)	0.5755 (3)	0.6632 (2)	0.0814 (10)
C10	1.1673 (7)	0.6086 (3)	0.71468 (18)	0.0783 (9)
H10	1.1688	0.5775	0.7616	0.094*
C11	1.3269 (6)	0.6865 (2)	0.69908 (16)	0.0695 (8)
H11	1.4343	0.7077	0.735	0.083*
C12	1.3254 (6)	0.7330 (2)	0.62925 (15)	0.0642 (7)
C13	1.1673 (8)	0.7010 (3)	0.57680 (19)	0.0836 (10)
H13	1.1667	0.7319	0.5298	0.1*
C14	1.0094 (7)	0.6231 (3)	0.5935 (2)	0.0892 (11)
H14	0.9025	0.6018	0.5575	0.107*
C15	1.6382 (7)	0.8487 (3)	0.6610 (2)	0.0891 (10)
H15A	1.73	0.904	0.6394	0.134*
H15B	1.7389	0.7919	0.6754	0.134*
H15C	1.5573	0.8749	0.704	0.134*
N1	0.9379 (4)	0.3862 (2)	0.66067 (15)	0.0790 (7)
O1	1.2662 (4)	0.2479 (2)	0.66466 (15)	0.0979 (8)
H1A	1.1921	0.2997	0.6782	0.147*
O2	1.4738 (5)	0.81229 (18)	0.60808 (11)	0.0847 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.082 (2)	0.070 (2)	0.0865 (18)	−0.0248 (18)	−0.0068 (17)	0.0110 (16)
C2	0.129 (4)	0.069 (2)	0.110 (3)	−0.037 (3)	0.019 (3)	−0.015 (2)

C3	0.138 (4)	0.055 (2)	0.135 (3)	−0.009 (3)	0.063 (3)	−0.006 (2)
C4	0.079 (2)	0.075 (2)	0.119 (3)	0.015 (2)	0.026 (2)	0.031 (2)
C5	0.0600 (15)	0.0640 (17)	0.0764 (16)	−0.0006 (15)	0.0024 (14)	0.0127 (14)
C6	0.0554 (14)	0.0459 (14)	0.0696 (14)	−0.0079 (12)	0.0013 (12)	0.0121 (12)
C7	0.0515 (13)	0.0542 (16)	0.0968 (18)	−0.0058 (14)	0.0057 (14)	0.0154 (15)
C8	0.091 (2)	0.068 (2)	0.165 (3)	−0.010 (2)	0.043 (3)	−0.030 (2)
C9	0.081 (2)	0.0504 (17)	0.113 (2)	0.0010 (16)	0.026 (2)	−0.0255 (18)
C10	0.099 (2)	0.0543 (16)	0.0814 (18)	0.0031 (19)	0.0169 (18)	−0.0043 (15)
C11	0.0839 (19)	0.0552 (16)	0.0694 (16)	0.0009 (16)	−0.0002 (15)	−0.0039 (13)
C12	0.0789 (18)	0.0457 (14)	0.0680 (14)	0.0075 (16)	0.0052 (14)	−0.0091 (12)
C13	0.108 (3)	0.072 (2)	0.0708 (16)	0.004 (2)	−0.0044 (18)	−0.0100 (15)
C14	0.095 (2)	0.073 (2)	0.099 (2)	0.001 (2)	−0.008 (2)	−0.030 (2)
C15	0.097 (2)	0.070 (2)	0.100 (2)	−0.015 (2)	0.008 (2)	−0.0039 (17)
N1	0.0726 (15)	0.0577 (15)	0.1068 (17)	−0.0101 (14)	0.0126 (15)	−0.0071 (14)
O1	0.0699 (13)	0.111 (2)	0.1132 (17)	0.0012 (16)	−0.0258 (14)	0.0017 (16)
O2	0.1129 (18)	0.0647 (13)	0.0765 (12)	−0.0104 (13)	0.0065 (13)	0.0056 (11)

Geometric parameters (Å, º)

C1—C2	1.381 (6)	C8—H8B	0.97
C1—C6	1.383 (4)	C9—C10	1.369 (5)
C1—H1	0.93	C9—C14	1.390 (5)
C2—C3	1.359 (7)	C10—C11	1.376 (5)
C2—H2	0.93	C10—H10	0.93
C3—C4	1.366 (6)	C11—C12	1.385 (4)
C3—H3	0.93	C11—H11	0.93
C4—C5	1.387 (5)	C12—C13	1.367 (5)
C4—H4	0.93	C12—O2	1.372 (4)
C5—O1	1.352 (4)	C13—C14	1.374 (5)
C5—C6	1.389 (4)	C13—H13	0.93
C6—C7	1.456 (4)	C14—H14	0.93
C7—N1	1.268 (4)	C15—O2	1.413 (4)
C7—H7	0.93	C15—H15A	0.96
C8—N1	1.464 (4)	C15—H15B	0.96
C8—C9	1.509 (5)	C15—H15C	0.96
C8—H8A	0.97	O1—H1A	0.82
C2—C1—C6	121.0 (4)	C10—C9—C14	117.7 (3)
C2—C1—H1	119.5	C10—C9—C8	121.2 (4)
C6—C1—H1	119.5	C14—C9—C8	121.0 (4)
C3—C2—C1	119.1 (4)	C9—C10—C11	122.0 (3)
C3—C2—H2	120.4	C9—C10—H10	119
C1—C2—H2	120.4	C11—C10—H10	119
C2—C3—C4	121.9 (4)	C10—C11—C12	119.2 (3)
C2—C3—H3	119	C10—C11—H11	120.4
C4—C3—H3	119	C12—C11—H11	120.4
C3—C4—C5	118.8 (4)	C13—C12—O2	116.0 (3)
C3—C4—H4	120.6	C13—C12—C11	119.9 (3)

C5—C4—H4	120.6	O2—C12—C11	124.1 (3)
O1—C5—C4	118.5 (3)	C12—C13—C14	120.0 (3)
O1—C5—C6	120.8 (3)	C12—C13—H13	120
C4—C5—C6	120.7 (3)	C14—C13—H13	120
C1—C6—C5	118.3 (3)	C13—C14—C9	121.2 (3)
C1—C6—C7	120.1 (3)	C13—C14—H14	119.4
C5—C6—C7	121.6 (3)	C9—C14—H14	119.4
N1—C7—C6	121.6 (3)	O2—C15—H15A	109.5
N1—C7—H7	119.2	O2—C15—H15B	109.5
C6—C7—H7	119.2	H15A—C15—H15B	109.5
N1—C8—C9	110.4 (3)	O2—C15—H15C	109.5
N1—C8—H8A	109.6	H15A—C15—H15C	109.5
C9—C8—H8A	109.6	H15B—C15—H15C	109.5
N1—C8—H8B	109.6	C7—N1—C8	118.9 (3)
C9—C8—H8B	109.6	C5—O1—H1A	109.5
H8A—C8—H8B	108.1	C12—O2—C15	117.8 (2)

C6—C1—C2—C3	0.5 (5)	C14—C9—C10—C11	0.4 (5)
C1—C2—C3—C4	−0.6 (6)	C8—C9—C10—C11	178.5 (3)
C2—C3—C4—C5	−1.1 (6)	C9—C10—C11—C12	−0.1 (5)
C3—C4—C5—O1	−178.3 (3)	C10—C11—C12—C13	−0.3 (4)
C3—C4—C5—C6	2.9 (5)	C10—C11—C12—O2	179.0 (3)
C2—C1—C6—C5	1.3 (4)	O2—C12—C13—C14	−179.0 (3)
C2—C1—C6—C7	−179.2 (3)	C11—C12—C13—C14	0.3 (5)
O1—C5—C6—C1	178.2 (3)	C12—C13—C14—C9	0.0 (5)
C4—C5—C6—C1	−3.0 (4)	C10—C9—C14—C13	−0.3 (5)
O1—C5—C6—C7	−1.3 (4)	C8—C9—C14—C13	−178.4 (3)
C4—C5—C6—C7	177.5 (3)	C6—C7—N1—C8	−179.6 (3)
C1—C6—C7—N1	179.4 (3)	C9—C8—N1—C7	−125.6 (4)
C5—C6—C7—N1	−1.0 (4)	C13—C12—O2—C15	179.2 (3)
N1—C8—C9—C10	−89.5 (4)	C11—C12—O2—C15	0.0 (4)
N1—C8—C9—C14	88.6 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*A*···N1	0.82	1.85	2.574 (3)	146
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