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(*E*)-2-[1-(2,4-Dimethoxyphenylimino)-ethyl]phenol

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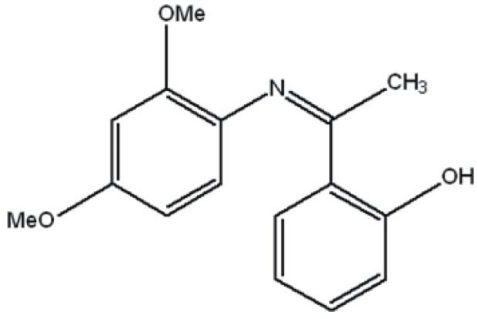
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.100; data-to-parameter ratio = 14.7.

In the title compound, $C_{16}H_{17}NO_3$, the dihedral angle between the two benzene rings is 66.20 (8)°. The molecular conformation is stabilized by an intramolecular O—H···N hydrogen bond formed between the phenol OH group and the Schiff base N atom.

Related literature

For background, see: Abilgaard *et al.* (2004); Allen *et al.* (1987); Dietz *et al.* (2000).



Experimental

Crystal data

$C_{16}H_{17}NO_3$
M_r = 271.31
Monoclinic, $P2_1/c$
a = 11.0449 (8) Å
b = 9.1047 (4) Å
c = 15.775 (1) Å
β = 118.190 (5)°
V = 1398.18 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
0.62 × 0.56 × 0.52 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.947, T_{max} = 0.955
16824 measured reflections
2754 independent reflections
2139 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.100
S = 1.01
2754 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···N1	0.976 (19)	1.588 (18)	2.5026 (15)	154.0 (19)

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2486).

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supplementary materials

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(*E*)-2-[1-(2,4-Dimethoxyphenylimino)ethyl]phenol

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Comment

Schiff bases derived from 2-hydroxyacetophenone are important ligands for transition metal complexes, especially for Ni and Cu (Dietz *et al.*, 2000). These Schiff bases are also interesting in hydrogen-bonding studies (Abilgaard *et al.*, 2004).

The title molecule, (I), (Fig. 1) adopts an *E* configuration with respect to the C═N double bond, with a C1—N1═C10—C11 torsion angle of −177.45 (14) ° and a C1—N1═C10 angle of 124.58 (12)°. In the hydroxyl group of the title compound, the C12—O3 bond distance is 1.3439 (18) Å. The C1—N1 and N1═C10 bond distances are 1.4230 (18) Å and 1.2856 (19) Å, respectively, in agreement with the mean literature values (Allen *et al.*, 1987). In the title compound, the two benzene rings make a dihedral angle of 66.20 (8)° with each other.

An intramolecular O—H···N hydrogen bond forms between the phenol OH group and the Schiff base N atom. The molecular structure is stabilized by this interaction and the crystal packing (Fig. 2) mainly by van der Waals forces.

Experimental

2-Hydroxyacetophenone (1.36 g, 1.2 ml, 10 mmol) and 2,4-dimethoxyaniline (0.79 g, 5.0 mmol) were dissolved in warm ethanol (10 ml). The reaction mixture was refluxed for 5 h and allowed to stand aside. Crude crystals were filtered off and washed with ethanol. The pure Schiff base was recrystallized as light brown crystals from ethanol (yield 98%, m.p. 644–646 K).

The IR spectrum showed absorption bands at 1612 cm^{-1} (C═N) and a signal for hydroxyl group at 3423 cm^{-1}. The ^{1}H-NMR spectrum showed signals for CH_3 at 1.92, OCH_3 at 3.62, 3.64, ArH at 6.23–7.36 p.p.m. and hydroxyl proton at 14.12 p.p.m.. The ^{13}C-NMR spectrum showed (CH_3) at 17.0 p.p.m., (OCH_3) at 54.87, 55.16 (ArC) at 103.82–132.09 p.p.m. (Ph—C—OH) at 162.36 and (C═N) 171.23 p.p.m.. The mass spectrum showed the base peak at *m/e* 271 and a peak at *m/e* 240 which is due to $C_{15}H_{14}NO_2$.

Refinement

The H atom of the hydroxy group was found from a difference Fourier map and refined freely. The other H atoms were geometrically placed and refined by using a riding model, with C—H = 0.93 − 0.96 Å and with U_{iso}(H) = 1.2U_{eq}($C_{aromatic}$) or 1.5U_{eq}(C_{methyl}).

Figures

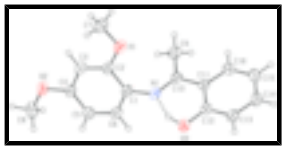

Fig. 1. View of (I) with 30% probability displacement ellipsoids for the non-hydrogen atoms.

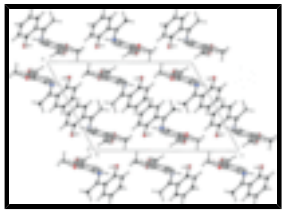

Fig. 2. The packing of the title compound, down the *b* axis.

(*E*)-2-[1-(2,4-Dimethoxyphenylimino)ethyl]phenol

Crystal data

$C_{16}H_{17}NO_3$	F_{000} = 576
M_r = 271.31	D_x = 1.289 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 23005 reflections
a = 11.0449 (8) Å	θ = 1.9–27.9º
b = 9.1047 (4) Å	μ = 0.09 mm^{-1}
c = 15.775 (1) Å	T = 296 K
β = 118.190 (5)º	Prism, light brown
V = 1398.18 (16) Å^3	0.62 × 0.56 × 0.52 mm
Z = 4	

Data collection

Stoe IPDS II diffractometer	2754 independent reflections
Monochromator: plane graphite	2139 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.055
T = 296 K	θ_{max} = 26.0º
ω scans	θ_{min} = 2.1º
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	h = −13→13
T_{min} = 0.947, T_{max} = 0.955	k = −11→11
16824 measured reflections	l = −19→19

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.049P)^2 + 0.1562P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.100$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.16$ e Å^{-3}
2754 reflections	$\Delta\rho_{min} = -0.14$ e Å^{-3}
187 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $FC^*=KFC[1+0.001XFC^2\Lambda^3/SIN(2\Theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.026 (2)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2$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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.81398 (12)	0.67302 (11)	0.30408 (8)	0.0624 (4)
O2	0.89590 (11)	1.18714 (11)	0.34470 (8)	0.0613 (4)
O3	0.82320 (11)	0.50782 (12)	0.59626 (7)	0.0604 (3)
N1	0.73912 (12)	0.66600 (12)	0.44954 (8)	0.0474 (4)
C1	0.76813 (14)	0.79933 (14)	0.41560 (9)	0.0460 (4)
C2	0.81382 (14)	0.80397 (14)	0.34636 (9)	0.0461 (4)
C3	0.85456 (14)	0.93581 (15)	0.32488 (10)	0.0492 (4)
C4	0.85139 (13)	1.06387 (14)	0.37117 (9)	0.0467 (4)
C5	0.80608 (15)	1.06124 (16)	0.43887 (10)	0.0538 (5)
C6	0.76698 (16)	0.92831 (16)	0.46068 (10)	0.0545 (5)
C7	0.8797 (2)	0.66865 (19)	0.24560 (12)	0.0676 (6)
C8	0.8879 (2)	1.32196 (17)	0.38609 (14)	0.0721 (6)
C9	0.52977 (16)	0.6165 (2)	0.29877 (10)	0.0651 (5)
C10	0.63442 (13)	0.58377 (14)	0.40028 (9)	0.0447 (4)
C11	0.61824 (13)	0.45310 (14)	0.44888 (9)	0.0435 (4)
C12	0.71375 (14)	0.42145 (14)	0.54554 (9)	0.0465 (4)
C13	0.69547 (17)	0.29878 (16)	0.59079 (11)	0.0566 (5)
C14	0.58574 (18)	0.20702 (16)	0.54196 (12)	0.0623 (6)
C15	0.49193 (17)	0.23502 (18)	0.44764 (12)	0.0634 (6)
C16	0.50768 (15)	0.35652 (16)	0.40257 (10)	0.0546 (5)
H3	0.88450	0.93870	0.27880	0.0590*

H3A	0.8146 (19)	0.584 (2)	0.5502 (13)	0.081 (5)*
H5	0.80190	1.14710	0.46930	0.0650*
H6	0.73880	0.92590	0.50770	0.0650*
H7A	0.97490	0.69400	0.28360	0.0810*
H7B	0.83630	0.73740	0.19370	0.0810*
H7C	0.87250	0.57150	0.22000	0.0810*
H8A	0.94260	1.31660	0.45470	0.0860*
H8B	0.79400	1.34130	0.37000	0.0860*
H8C	0.92150	1.39960	0.36170	0.0860*
H9A	0.54460	0.55340	0.25580	0.0780*
H9B	0.53830	0.71710	0.28420	0.0780*
H9C	0.43940	0.60000	0.29130	0.0780*
H13	0.75810	0.27890	0.65450	0.0680*
H14	0.57450	0.12510	0.57280	0.0750*
H15	0.41820	0.17170	0.41470	0.0760*
H16	0.44280	0.37540	0.33920	0.0660*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0874 (8)	0.0495 (6)	0.0738 (7)	0.0032 (5)	0.0573 (6)	0.0023 (5)
O2	0.0742 (7)	0.0501 (6)	0.0724 (7)	−0.0040 (5)	0.0452 (6)	0.0095 (5)
O3	0.0609 (6)	0.0649 (7)	0.0453 (5)	−0.0165 (5)	0.0168 (5)	0.0084 (5)
N1	0.0539 (7)	0.0478 (6)	0.0452 (6)	−0.0039 (5)	0.0274 (5)	0.0045 (5)
C1	0.0480 (7)	0.0491 (8)	0.0439 (7)	−0.0010 (6)	0.0241 (6)	0.0075 (6)
C2	0.0493 (7)	0.0468 (7)	0.0458 (7)	0.0049 (6)	0.0255 (6)	0.0056 (6)
C3	0.0529 (8)	0.0547 (8)	0.0497 (7)	0.0052 (6)	0.0323 (6)	0.0103 (6)
C4	0.0447 (7)	0.0475 (7)	0.0485 (7)	0.0005 (6)	0.0226 (6)	0.0102 (6)
C5	0.0645 (9)	0.0495 (8)	0.0546 (8)	−0.0038 (6)	0.0341 (7)	−0.0012 (6)
C6	0.0665 (9)	0.0574 (9)	0.0512 (7)	−0.0059 (7)	0.0374 (7)	0.0009 (6)
C7	0.0900 (12)	0.0635 (10)	0.0707 (10)	0.0175 (8)	0.0555 (10)	0.0090 (8)
C8	0.0801 (11)	0.0478 (9)	0.0975 (13)	−0.0058 (8)	0.0495 (10)	0.0060 (8)
C9	0.0596 (9)	0.0817 (11)	0.0478 (8)	−0.0058 (8)	0.0204 (7)	0.0110 (7)
C10	0.0469 (7)	0.0524 (8)	0.0413 (6)	0.0005 (6)	0.0262 (6)	0.0003 (6)
C11	0.0495 (7)	0.0463 (7)	0.0423 (7)	−0.0031 (5)	0.0280 (6)	−0.0037 (5)
C12	0.0512 (7)	0.0483 (7)	0.0458 (7)	−0.0053 (6)	0.0277 (6)	−0.0013 (6)
C13	0.0673 (9)	0.0564 (9)	0.0532 (8)	−0.0015 (7)	0.0343 (7)	0.0078 (6)
C14	0.0808 (11)	0.0474 (8)	0.0763 (10)	−0.0089 (7)	0.0517 (9)	0.0016 (7)
C15	0.0680 (10)	0.0570 (9)	0.0743 (10)	−0.0209 (7)	0.0412 (9)	−0.0148 (8)
C16	0.0563 (8)	0.0594 (9)	0.0512 (8)	−0.0097 (7)	0.0280 (7)	−0.0102 (6)

Geometric parameters (Å, °)

O1—C2	1.3666 (17)	C13—C14	1.371 (3)
O1—C7	1.419 (3)	C14—C15	1.377 (2)
O2—C4	1.3673 (18)	C15—C16	1.370 (2)
O2—C8	1.413 (2)	C3—H3	0.9300
O3—C12	1.3439 (18)	C5—H5	0.9300
O3—H3A	0.976 (19)	C6—H6	0.9300

N1—C1	1.4230 (18)	C7—H7A	0.9600
N1—C10	1.2856 (19)	C7—H7B	0.9600
C1—C6	1.376 (2)	C7—H7C	0.9600
C1—C2	1.404 (2)	C8—H8A	0.9600
C2—C3	1.379 (2)	C8—H8B	0.9600
C3—C4	1.3849 (19)	C8—H8C	0.9600
C4—C5	1.377 (2)	C9—H9A	0.9600
C5—C6	1.382 (2)	C9—H9B	0.9600
C9—C10	1.4968 (19)	C9—H9C	0.9600
C10—C11	1.4713 (19)	C13—H13	0.9300
C11—C16	1.398 (2)	C14—H14	0.9300
C11—C12	1.4146 (18)	C15—H15	0.9300
C12—C13	1.391 (2)	C16—H16	0.9300
C2—O1—C7	117.45 (13)	C4—C5—H5	121.00
C4—O2—C8	117.52 (14)	C6—C5—H5	121.00
C12—O3—H3A	103.2 (12)	C1—C6—H6	119.00
C1—N1—C10	124.58 (12)	C5—C6—H6	119.00
N1—C1—C6	118.35 (13)	O1—C7—H7A	109.00
C2—C1—C6	118.10 (13)	O1—C7—H7B	109.00
N1—C1—C2	123.10 (12)	O1—C7—H7C	109.00
O1—C2—C3	124.31 (14)	H7A—C7—H7B	110.00
C1—C2—C3	119.76 (12)	H7A—C7—H7C	109.00
O1—C2—C1	115.94 (12)	H7B—C7—H7C	109.00
C2—C3—C4	120.71 (14)	O2—C8—H8A	109.00
O2—C4—C5	124.46 (12)	O2—C8—H8B	109.00
C3—C4—C5	120.21 (13)	O2—C8—H8C	110.00
O2—C4—C3	115.32 (13)	H8A—C8—H8B	109.00
C4—C5—C6	118.62 (14)	H8A—C8—H8C	109.00
C1—C6—C5	122.58 (15)	H8B—C8—H8C	109.00
N1—C10—C11	116.87 (12)	C10—C9—H9A	109.00
C9—C10—C11	119.74 (13)	C10—C9—H9B	109.00
N1—C10—C9	123.39 (13)	C10—C9—H9C	109.00
C10—C11—C16	121.83 (12)	H9A—C9—H9B	109.00
C12—C11—C16	117.23 (12)	H9A—C9—H9C	110.00
C10—C11—C12	120.94 (12)	H9B—C9—H9C	110.00
O3—C12—C13	118.18 (12)	C12—C13—H13	120.00
C11—C12—C13	120.11 (14)	C14—C13—H13	120.00
O3—C12—C11	121.71 (12)	C13—C14—H14	120.00
C12—C13—C14	120.36 (14)	C15—C14—H14	120.00
C13—C14—C15	120.58 (15)	C14—C15—H15	120.00
C14—C15—C16	119.68 (16)	C16—C15—H15	120.00
C11—C16—C15	122.03 (14)	C11—C16—H16	119.00
C2—C3—H3	120.00	C15—C16—H16	119.00
C4—C3—H3	120.00		
C7—O1—C2—C1	−170.09 (14)	O2—C4—C5—C6	−178.43 (14)
C7—O1—C2—C3	10.1 (2)	C3—C4—C5—C6	1.3 (2)
C8—O2—C4—C5	−3.5 (2)	C4—C5—C6—C1	−1.8 (2)
C8—O2—C4—C3	176.74 (15)	N1—C10—C11—C12	0.4 (2)

C10—N1—C1—C2	−72.2 (2)	N1—C10—C11—C16	179.48 (15)
C1—N1—C10—C11	−177.45 (14)	C9—C10—C11—C12	−178.44 (14)
C1—N1—C10—C9	1.4 (2)	C9—C10—C11—C16	0.6 (2)
C10—N1—C1—C6	115.74 (17)	C10—C11—C12—O3	−0.8 (2)
N1—C1—C2—C3	−172.73 (14)	C10—C11—C12—C13	178.90 (15)
N1—C1—C6—C5	173.90 (15)	C16—C11—C12—O3	−179.83 (14)
C6—C1—C2—C3	−0.6 (2)	C16—C11—C12—C13	−0.2 (2)
C2—C1—C6—C5	1.4 (2)	C10—C11—C16—C15	−179.76 (16)
N1—C1—C2—O1	7.4 (2)	C12—C11—C16—C15	−0.7 (2)
C6—C1—C2—O1	179.57 (14)	O3—C12—C13—C14	−179.74 (16)
O1—C2—C3—C4	−179.95 (15)	C11—C12—C13—C14	0.6 (3)
C1—C2—C3—C4	0.2 (2)	C12—C13—C14—C15	−0.2 (3)
C2—C3—C4—O2	179.18 (14)	C13—C14—C15—C16	−0.7 (3)
C2—C3—C4—C5	−0.6 (2)	C14—C15—C16—C11	1.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···N1	0.976 (19)	1.588 (18)	2.5026 (15)	154.0 (19)

Fig. 1

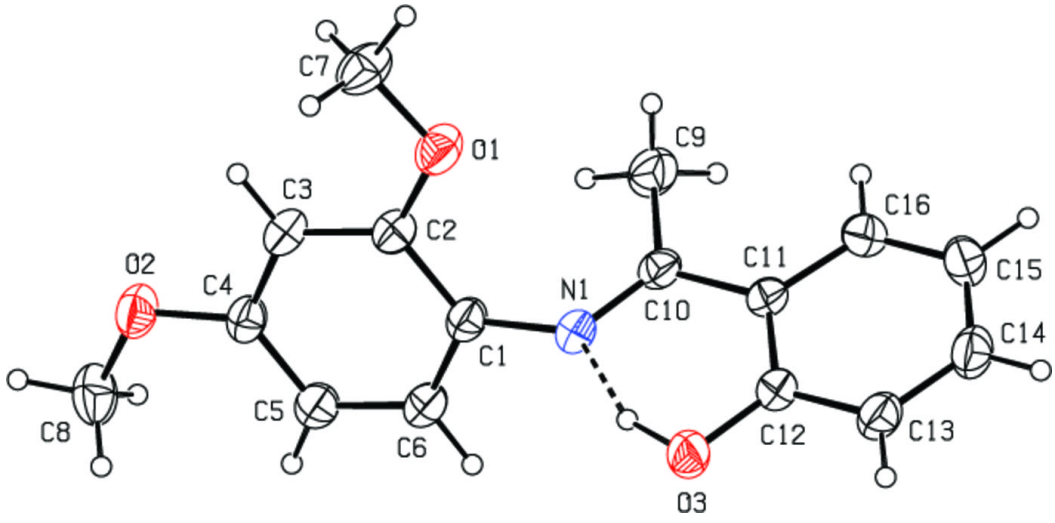

Fig. 2