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(*E*)-2-[4-(Dimethylamino)phenyliminomethyl]-6-methylphenol

Zarife Sibel Gül,[a]* Ferda Erşahin,[b] Erbil Ağar[b] and Şamil Işık[a]

[a]Department of Physics, Arts and Sciences Faculty, Ondokuz Mayıs University, 55139 Samsun, Turkey, and [b]Department of Chemistry, Arts and Sciences Faculty, Ondokuz Mayıs University, 55139 Samsun, Turkey
Correspondence e-mail: sgul@omu.edu.tr

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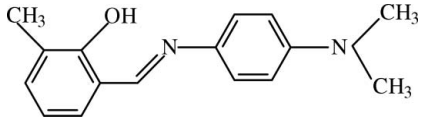
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.044; wR factor = 0.112; data-to-parameter ratio = 15.7.

The title compound, $C_{16}H_{18}N_2O$, a Schiff base, crystallizes in the phenol–imine tautomeric form, with a strong intramolecular O—H···N hydrogen bond which forms an almost planar ring.

Related literature

Schiff base compounds can be classified by their photochromic and thermochromic characteristics (Cohen *et al.*, 1964; Hadjoudis *et al.*, 1987).

For related literature, see: Bernstein *et al.* (1995); Gül *et al.* (2007); Garnovskii *et al.* (1993); Karadayı *et al.* (2003); Lozier *et al.* (1975); Williams (1972); Xu *et al.* (1994); Yüce *et al.* (2004).



Experimental

Crystal data

$C_{16}H_{18}N_2O$
M_r = 254.32
Monoclinic, $P2_1/c$
a = 8.3899 (9) Å
b = 6.0651 (4) Å
c = 28.305 (3) Å
β = 100.502 (9)°
V = 1416.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.80 × 0.42 × 0.04 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration from crystal shape (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.952, T_{max} = 0.996
13978 measured reflections
2784 independent reflections
1105 reflections with $I > 2\sigma(I)$
R_{int} = 0.085

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.112
S = 0.82
2784 reflections
177 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.99 (4)	1.62 (4)	2.574 (3)	159 (3)

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: LX2009).

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supplementary materials

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(*E*)-2-[4-(Dimethylamino)phenyliminomethyl]-6-methylphenol

Z. S. Gül, F. Ersahin, E. Agar and S. Isik

Comment

Most Schiff bases have antibacterial, anticancer, antiinflammatory and antitoxic properties (Williams, 1972). In addition, Schiff bases are important in diverse fields of chemistry and biochemistry owing to their biological activites (Lozier *et al.*, 1975; Garnovskii *et al.*, 1993). Photochromism and thermochromism are also characteristics of these materials and arise *via* H-atom transfer from the hydroxy O atom to the N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994). These are two types of intra molecular hydrogen bonds in Schiff bases, in keto-amine (N—H···O) and phenol-imine (N···H—O) tautomeric forms. The present X-ray investigation shows that the title compound, (I), exists in the phenol-imine form (Fig.1).

Our investigations show that all bond lengths and angles are normal. The C8—N1 and C1—C7 bond lengths are 1.412 (2) and 1.441 (3) Å, respectively and agree with the corresponding distances in 1-{4-[(2-hydroxy-benzylidene)amino] phenyl}ethanone [1.4138 (17) and 1.4428 (18) Å; Yüce *et al.*, 2004]. The N1═C7 bond length of 1.280 (2) Å is typical of a double bond, similar to the corresponding bond length in *N*-[3,5-Bis(trifluoromethyl)phenyl]salicylaldimine [1.276 (4) Å; Karadayı *et al.*, 2003]. The O1—C6 distance of 1.350 (3) Å is close to the value of 1.352 (3) Å in (*E*)-2-[(3-trifluoromethylphenylimino)methyl]-4-methylphenol (Gül *et al.*, 2007). The dihedral angle between the rings formed by atoms C1—C6 and C8—C13 is 7.86 (13)°. Fig.1 also shows a strong intramolecular hydrogen bond (O1—H1···N1) can be described as an S(6) motif (Bernstein *et al.*, 1995). The O1—N1 distance of 2.574 (3) Å is comparable to those observed for analogous hydrogen bonds in 1-{4-[(2-hydroxy-benzylidene)amino]phenyl}ethanone [2.5941 (15) Å; Yüce *et al.*, 2004].

Experimental

The compound (*E*)-2-[(4-*N*,*N*-dimethylaminophenylimino)methyl] -6-methylphenol was prepared by reflux a mixture of a solution containing 3-methylsalicylaldehyde (0.1 ml 0.82 mmol) in 20 ml e thanol and a solution containing 4-*N*,*N*-dimethylphenylendiamin (0.14 g 0.82 mmol) in 20 ml e thanol. The reaction mixture was stirred for 1 h under reflux. The crystals of (*E*)-2-[(4-*N*,*N*-dimethylaminophenylimino)methyl]-6-methylphenol suitable for X-ray analysis were obtained from ethylalcohol by slow evaporation (yield % 38; m.p. 378–379 K).

Refinement

The H1 atom was located in a difference map and refined freely. All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C).

Figures

Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 40% probability level for non-H atoms.

(*E*)-2-[4-(Dimethylamino)phenyliminomethyl]-6-methylphenol

Crystal data

$C_{16}H_{18}N_2O$	F_{000} = 544
M_r = 254.32	D_x = 1.193 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 6157 reflections
a = 8.3899 (9) Å	θ = 2.2–29.1º
b = 6.0651 (4) Å	μ = 0.08 mm^{-1}
c = 28.305 (3) Å	T = 296 K
β = 100.502 (9)º	Prism, yellow
V = 1416.2 (2) Å^3	0.80 × 0.42 × 0.04 mm
Z = 4	

Data collection

Stoe IPDS II diffractometer	2784 independent reflections
Radiation source: fine-focus sealed tube	1105 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.085
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 26.0º
T = 296 K	θ_{min} = 2.5º
ω scans	h = −10→10
Absorption correction: integration from crystal shape (X-RED32; Stoe & Cie, 2002)	k = −7→7
T_{min} = 0.952, T_{max} = 0.996	l = −34→34
13978 measured reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.112	$\Delta\rho_{max}$ = 0.10 e Å^{-3}
S = 0.82	$\Delta\rho_{min}$ = −0.10 e Å^{-3}
2784 reflections	Extinction correction: none
177 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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	0.6175 (2)	0.6277 (4)	0.88499 (8)	0.0785 (6)
C2	0.7394 (3)	0.7759 (5)	0.90267 (10)	0.1035 (8)
H2	0.7608	0.8932	0.8836	0.124*
C3	0.8291 (3)	0.7513 (6)	0.94819 (12)	0.1255 (11)
H3	0.9114	0.8504	0.9598	0.151*
C4	0.7955 (4)	0.5784 (7)	0.97624 (10)	0.1163 (11)
H4	0.8567	0.5629	1.0069	0.140*
C5	0.6757 (3)	0.4286 (5)	0.96084 (9)	0.1018 (9)
C6	0.5880 (3)	0.4526 (5)	0.91436 (8)	0.0836 (7)
C7	0.5235 (2)	0.6566 (4)	0.83744 (8)	0.0783 (6)
H7	0.5445	0.7773	0.8192	0.094*
C8	0.3122 (2)	0.5455 (4)	0.77405 (7)	0.0651 (5)
C9	0.3143 (3)	0.7199 (4)	0.74297 (8)	0.0810 (6)
H9	0.3916	0.8301	0.7508	0.097*
C10	0.2044 (3)	0.7343 (4)	0.70062 (8)	0.0805 (6)
H10	0.2094	0.8538	0.6804	0.097*
C11	0.0858 (2)	0.5740 (3)	0.68735 (7)	0.0659 (5)
C12	0.0882 (2)	0.3937 (3)	0.71795 (7)	0.0716 (6)
H12	0.0146	0.2793	0.7098	0.086*
C13	0.1987 (2)	0.3840 (3)	0.76009 (8)	0.0734 (6)
H13	0.1966	0.2627	0.7801	0.088*
C14	−0.0300 (3)	0.7795 (4)	0.61455 (9)	0.1074 (9)
H14A	−0.1177	0.7648	0.5877	0.161*
H14B	0.0708	0.7862	0.6031	0.161*
H14C	−0.0441	0.9121	0.6318	0.161*
C15	−0.1539 (3)	0.4305 (4)	0.63341 (9)	0.0966 (7)
H15A	−0.2220	0.4710	0.6036	0.145*
H15B	−0.2178	0.4229	0.6583	0.145*
H15C	−0.1057	0.2893	0.6300	0.145*
C16	0.6370 (4)	0.2447 (6)	0.99256 (10)	0.1431 (13)
H16A	0.7109	0.2496	1.0227	0.215*
H16B	0.6473	0.1057	0.9772	0.215*
H16C	0.5280	0.2615	0.9980	0.215*

N1	0.41195 (19)	0.5207 (3)	0.81961 (6)	0.0732 (5)
N2	−0.0287 (2)	0.5925 (3)	0.64594 (6)	0.0781 (5)
O1	0.4702 (2)	0.3038 (3)	0.89906 (8)	0.1108 (6)
H1	0.439 (4)	0.354 (5)	0.8653 (14)	0.169 (13)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0598 (13)	0.1073 (18)	0.0686 (15)	0.0066 (13)	0.0119 (11)	−0.0091 (14)
C2	0.0801 (17)	0.140 (2)	0.087 (2)	−0.0121 (16)	0.0073 (15)	−0.0164 (16)
C3	0.090 (2)	0.182 (3)	0.095 (2)	−0.002 (2)	−0.0073 (18)	−0.040 (2)
C4	0.087 (2)	0.184 (3)	0.0726 (18)	0.039 (2)	−0.0004 (16)	−0.026 (2)
C5	0.0864 (17)	0.144 (3)	0.0718 (18)	0.0399 (18)	0.0065 (14)	−0.0058 (18)
C6	0.0676 (14)	0.111 (2)	0.0711 (16)	0.0220 (14)	0.0087 (12)	−0.0001 (15)
C7	0.0625 (13)	0.1002 (17)	0.0728 (16)	0.0053 (13)	0.0140 (12)	0.0016 (12)
C8	0.0571 (11)	0.0760 (14)	0.0612 (13)	0.0012 (11)	0.0084 (10)	0.0033 (11)
C9	0.0691 (14)	0.0878 (16)	0.0826 (16)	−0.0151 (11)	0.0044 (12)	0.0120 (13)
C10	0.0778 (14)	0.0846 (15)	0.0757 (15)	−0.0138 (13)	0.0048 (12)	0.0241 (13)
C11	0.0644 (12)	0.0735 (14)	0.0592 (12)	0.0009 (11)	0.0101 (10)	0.0012 (11)
C12	0.0739 (13)	0.0657 (13)	0.0717 (14)	−0.0097 (11)	0.0044 (11)	0.0089 (12)
C13	0.0774 (13)	0.0722 (14)	0.0672 (13)	−0.0004 (12)	0.0039 (11)	0.0151 (11)
C14	0.1044 (19)	0.115 (2)	0.0925 (19)	−0.0050 (15)	−0.0103 (15)	0.0396 (16)
C15	0.0992 (16)	0.0915 (16)	0.0869 (17)	−0.0078 (15)	−0.0150 (13)	−0.0023 (14)
C16	0.165 (3)	0.183 (3)	0.078 (2)	0.061 (2)	0.014 (2)	0.032 (2)
N1	0.0570 (9)	0.0914 (13)	0.0684 (11)	0.0052 (10)	0.0045 (9)	0.0014 (10)
N2	0.0798 (11)	0.0818 (12)	0.0674 (11)	−0.0053 (10)	−0.0008 (9)	0.0096 (10)
O1	0.1058 (14)	0.1237 (15)	0.0945 (14)	−0.0067 (11)	−0.0040 (11)	0.0253 (12)

Geometric parameters (Å, °)

C1—C7	1.441 (3)	C10—C11	1.393 (3)
C6—O1	1.350 (3)	C10—H10	0.9300
C7—N1	1.280 (2)	C11—N2	1.378 (2)
C8—N1	1.412 (2)	C11—C12	1.393 (3)
C1—C2	1.385 (3)	C12—C13	1.372 (3)
C1—C6	1.398 (3)	C12—H12	0.9300
C2—C3	1.376 (4)	C13—H13	0.9300
C2—H2	0.9300	C14—N2	1.439 (3)
C3—C4	1.375 (4)	C14—H14A	0.9600
C3—H3	0.9300	C14—H14B	0.9600
C4—C5	1.365 (4)	C14—H14C	0.9600
C4—H4	0.9300	C15—N2	1.435 (3)
C5—C6	1.393 (3)	C15—H15A	0.9600
C5—C16	1.504 (4)	C15—H15B	0.9600
C7—H7	0.9300	C15—H15C	0.9600
C8—C13	1.373 (3)	C16—H16A	0.9600
C8—C9	1.378 (3)	C16—H16B	0.9600
C9—C10	1.375 (3)	C16—H16C	0.9600
C9—H9	0.9300	O1—H1	0.99 (4)

C2—C1—C6	118.5 (2)	N2—C11—C10	121.7 (2)
C2—C1—C7	120.0 (3)	C12—C11—C10	116.83 (19)
C6—C1—C7	121.4 (2)	C13—C12—C11	120.4 (2)
C3—C2—C1	120.6 (3)	C13—C12—H12	119.8
C3—C2—H2	119.7	C11—C12—H12	119.8
C1—C2—H2	119.7	C12—C13—C8	122.9 (2)
C4—C3—C2	119.2 (3)	C12—C13—H13	118.6
C4—C3—H3	120.4	C8—C13—H13	118.6
C2—C3—H3	120.4	N2—C14—H14A	109.5
C5—C4—C3	122.6 (3)	N2—C14—H14B	109.5
C5—C4—H4	118.7	H14A—C14—H14B	109.5
C3—C4—H4	118.7	N2—C14—H14C	109.5
C4—C5—C6	117.6 (3)	H14A—C14—H14C	109.5
C4—C5—C16	122.0 (3)	H14B—C14—H14C	109.5
C6—C5—C16	120.4 (3)	N2—C15—H15A	109.5
O1—C6—C5	117.6 (3)	N2—C15—H15B	109.5
O1—C6—C1	121.1 (2)	H15A—C15—H15B	109.5
C5—C6—C1	121.3 (3)	N2—C15—H15C	109.5
N1—C7—C1	121.7 (2)	H15A—C15—H15C	109.5
N1—C7—H7	119.1	H15B—C15—H15C	109.5
C1—C7—H7	119.1	C5—C16—H16A	109.5
C13—C8—C9	116.9 (2)	C5—C16—H16B	109.5
C13—C8—N1	116.8 (2)	H16A—C16—H16B	109.5
C9—C8—N1	126.2 (2)	C5—C16—H16C	109.5
C10—C9—C8	121.4 (2)	H16A—C16—H16C	109.5
C10—C9—H9	119.3	H16B—C16—H16C	109.5
C8—C9—H9	119.3	C7—N1—C8	124.1 (2)
C9—C10—C11	121.5 (2)	C11—N2—C15	121.32 (19)
C9—C10—H10	119.2	C11—N2—C14	121.0 (2)
C11—C10—H10	119.2	C15—N2—C14	117.7 (2)
N2—C11—C12	121.5 (2)	C6—O1—H1	98.8 (19)
C6—C1—C2—C3	−0.1 (3)	N1—C8—C9—C10	−175.8 (2)
C7—C1—C2—C3	179.4 (2)	C8—C9—C10—C11	0.3 (3)
C1—C2—C3—C4	−0.6 (4)	C9—C10—C11—N2	177.2 (2)
C2—C3—C4—C5	−0.1 (4)	C9—C10—C11—C12	−2.8 (3)
C3—C4—C5—C6	1.4 (4)	N2—C11—C12—C13	−176.96 (19)
C3—C4—C5—C16	−178.0 (3)	C10—C11—C12—C13	3.0 (3)
C4—C5—C6—O1	179.6 (2)	C11—C12—C13—C8	−0.9 (3)
C16—C5—C6—O1	−1.0 (3)	C9—C8—C13—C12	−1.6 (3)
C4—C5—C6—C1	−2.0 (3)	N1—C8—C13—C12	176.32 (18)
C16—C5—C6—C1	177.3 (2)	C1—C7—N1—C8	177.48 (18)
C2—C1—C6—O1	179.7 (2)	C13—C8—N1—C7	179.63 (18)
C7—C1—C6—O1	0.2 (3)	C9—C8—N1—C7	−2.7 (3)
C2—C1—C6—C5	1.5 (3)	C12—C11—N2—C15	2.2 (3)
C7—C1—C6—C5	−178.1 (2)	C10—C11—N2—C15	−177.8 (2)
C2—C1—C7—N1	178.7 (2)	C12—C11—N2—C14	−179.94 (19)
C6—C1—C7—N1	−1.8 (3)	C10—C11—N2—C14	0.1 (3)
C13—C8—C9—C10	1.9 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.99 (4)	1.62 (4)	2.574 (3)	159 (3)

Fig. 1