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5-Diethylamino-2-{(*E*)-[(3-iodophenyl)-imino]methyl}phenol

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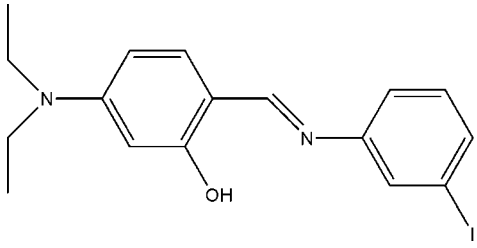
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.008 Å; R factor = 0.037; wR factor = 0.074; data-to-parameter ratio = 17.0.

The title Schiff base, $C_{17}H_{19}IN_2O$, is not planar, displaying a dihedral angle of 34.9 (2)° between the two aromatic rings. The molecular conformation allows the formation of a strong intramolecular O—H···N hydrogen bond with graph-set motif $S(6)$ between the hydroxy group and the imine N atom.

Related literature

For Schiff base tautomerism, see: Cohen *et al.* (1964); Hadjoudis *et al.* (1987). For the biological properties of Schiff bases, see: Dao *et al.* (2000). For related structures, see: Gül, Ağar & Işık (2007); Gül, Erşahin, Ağar & Işık (2007); Pekdemir *et al.* (2012); Yüce *et al.* (2004); Demirtaş *et al.* (2011). For the classification of hydrogen-bonding patterns, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{17}H_{19}IN_2O$
M_r = 394.24
Orthorhombic, $P2_12_12_1$
a = 6.6999 (6) Å
b = 15.248 (2) Å
c = 16.1195 (15) Å
V = 1646.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.95 mm^{-1}
T = 296 K
0.49 × 0.34 × 0.21 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.451, T_{max} = 0.603
6072 measured reflections
3225 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.074
S = 0.86
3225 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}
Absolute structure: Flack (1983), 1355 Friedel pairs
Flack parameter: −0.02 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.82	1.85	2.577 (6)	147

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, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2429).

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supplementary materials

Acta Cryst. (2012). E**68**, o1963 [doi:10.1107/S1600536812022556]

5-Diethylamino-2-{(*E*)-[(3-iodophenyl)imino]methyl}phenol

Hilal Vesek, Canan Kazak, Erbil Ağar and Sümeyye Gümüş

Comment

Schiff base compounds are used in many different areas. Generally, they exhibit biological activity: anti-bacterial and anti-cancer properties were demonstrated (Dao *et al.*, 2000). Thermochromic and photochromic Schiff base compounds can be classified on the basis of their specific characteristics (Cohen *et al.*, 1964): intermolecular hydrogen bonds may be formed in two different ways. Chromic action is strongly related to the tautomerization between the O—H···N═C—C═C (enolimino) and —C═ O···H—N—C═C—C (ketoamino) tautomeric forms (Hadjoudis *et al.*, 1987). The title compound is stabilized in the phenol-imine tautomeric form (Fig. 1).

The C1—N1 bond length, 1.407 (7) Å, is in agreement with the distance reported for 2-[(*E*)-(naphthalen-2-ylimino)-methyl]-4-(trifluoromethoxy)phenol [1.417 (2) Å, Pekdemir *et al.*, 2012] and 1-{4-[(2-hydroxybenzylidene)amino]-phenyl}ethanone [1.4138 (17) Å, Yüce *et al.*, 2004]. The C7═N1 bond length of 1.292 (7) Å is also comparable to the imine double bond found in (*E*)-4-bromo-2-[(2-hydroxy-5-methylphenyl)iminomethy]phenol [1.289 (6) Å, Gül, Ağar & Işık, 2007]. Figure 1 also shows a strong intramolecular hydrogen bond O1—H1···N1, which can be described as an *S*(6) motif (Bernstein *et al.*, 1995). The O1···N1 separation of 2.577 (6) Å is comparable to that observed for similar hydrogen bonds in related Schiff bases (Gül, Erşahin, Ağar & Işık, 2007). The C3—I1 bond length, 2.114 (5) Å, is in agreement with other C—I bonds, for example in 2-(2-iodophenyl)isoindoline-1,3-dione [2.094 (3) Å; Demirtaş *et al.*, 2011]. The title molecule is not planar, displaying a dihedral angle of 34.9 (2)° between the two aromatic rings.

Experimental

The title compound was prepared by refluxing for 1 h. a mixture of 4-(diethylamino)-2-hydroxybenzaldehyde (0.022 g, 0.11 mmol) in ethanol (20 ml) and 3-iodoaniline (0.025 g, 0.11 mmol) in ethanol (20 ml). Crystals suitable for X-ray analysis were obtained from ethanol by slow evaporation (yield: 72%, m.p. 394–395 K).

Refinement

The H atom of the hydroxy group was refined with the O1—H1 bond length constrained to 0.82 Å and U_{iso}(H1) = 1.5U_{eq}(O1). All other H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C—H = 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). The refinement of the Flack parameter (Flack, 1983) is based on 1355 measured Friedel pairs.

Computing details

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA* (Stoe & Cie, 2002); data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Spek, 2009).

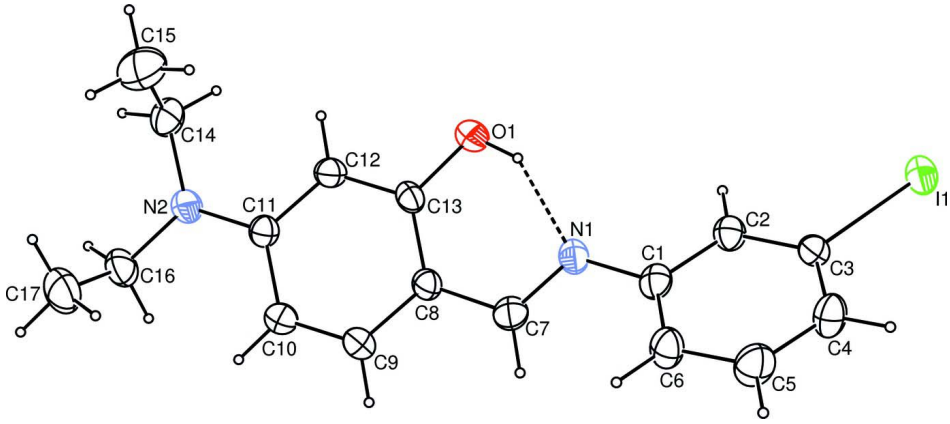

Figure 1

The molecular structure of the title compound, showing displacement ellipsoids at the 30% probability level.

5-Diethylamino-2-{(*E*)-[(3-iodophenyl)imino]methyl}phenol

Crystal data

$C_{17}H_{19}IN_2O$
M_r = 394.24
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
a = 6.6999 (6) Å
b = 15.248 (2) Å
c = 16.1195 (15) Å
V = 1646.7 (3) Å^3
Z = 4
F(000) = 784
D_x = 1.590 Mg m^{-3}
Melting point: 394 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 8061 reflections
θ = 1.8–28.1°
μ = 1.95 mm^{-1}
T = 296 K
Prism, yellow
0.49 × 0.34 × 0.21 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
rotation method scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.451, T_{max} = 0.603
6072 measured reflections
3225 independent reflections
2417 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 26.0°, θ_{min} = 1.8°
h = −6→8
k = −15→19
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.074
S = 0.86
3225 reflections
190 parameters
0 restraints
0 constraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}
Absolute structure: Flack (1983), 1355 Friedel pairs
Flack parameter: −0.02 (3)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.5355 (9)	0.7994 (3)	0.3130 (3)	0.0424 (14)
C2	0.6547 (9)	0.8639 (3)	0.2779 (3)	0.0438 (13)
H2	0.7869	0.8699	0.2946	0.053*
C3	0.5784 (8)	0.9186 (3)	0.2188 (3)	0.0411 (13)
C4	0.3846 (10)	0.9108 (4)	0.1905 (4)	0.0539 (16)
H4	0.3353	0.9477	0.1494	0.065*
C5	0.2675 (12)	0.8468 (4)	0.2254 (4)	0.0648 (16)
H5	0.1361	0.8409	0.2077	0.078*
C6	0.3395 (9)	0.7908 (4)	0.2860 (4)	0.0513 (15)
H6	0.2573	0.7478	0.3085	0.062*
C7	0.5263 (10)	0.7053 (4)	0.4284 (3)	0.0463 (16)
H7	0.3934	0.7205	0.4366	0.056*
C8	0.6183 (8)	0.6397 (4)	0.4808 (4)	0.0398 (14)
C9	0.5079 (9)	0.5976 (4)	0.5432 (4)	0.0470 (14)
H9	0.3765	0.6148	0.5522	0.056*
C10	0.5856 (9)	0.5330 (4)	0.5909 (3)	0.0474 (15)
H10	0.5071	0.5067	0.6314	0.057*
C11	0.7872 (8)	0.5048 (3)	0.5794 (3)	0.0396 (12)
C12	0.8970 (8)	0.5476 (4)	0.5182 (3)	0.0429 (13)
H12	1.0285	0.5305	0.5091	0.052*
C13	0.8187 (8)	0.6140 (4)	0.4706 (3)	0.0382 (14)
C14	1.0628 (11)	0.4029 (4)	0.6072 (4)	0.0602 (17)
H14A	1.1138	0.3722	0.6555	0.072*
H14B	1.1530	0.4512	0.5956	0.072*
C15	1.0651 (14)	0.3412 (6)	0.5345 (5)	0.098 (3)
H15A	1.1984	0.3200	0.5259	0.147*
H15B	1.0204	0.3715	0.4858	0.147*
H15C	0.9779	0.2926	0.5455	0.147*
C16	0.7536 (12)	0.3977 (4)	0.6930 (3)	0.0594 (15)
H16A	0.6713	0.4420	0.7194	0.071*
H16B	0.8452	0.3752	0.7345	0.071*
C17	0.6208 (11)	0.3235 (5)	0.6640 (6)	0.085 (2)
H17A	0.5497	0.2997	0.7105	0.127*
H17B	0.7012	0.2785	0.6392	0.127*
H17C	0.5273	0.3454	0.6239	0.127*
I1	0.76828 (6)	1.01529 (2)	0.16772 (2)	0.05438 (13)
N1	0.6279 (7)	0.7428 (3)	0.3703 (3)	0.0431 (11)
N2	0.8680 (7)	0.4386 (3)	0.6273 (3)	0.0478 (12)
O1	0.9360 (6)	0.6522 (3)	0.4129 (2)	0.0532 (11)
H1	0.8727	0.6905	0.3888	0.080*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.056 (3)	0.032 (3)	0.039 (3)	0.004 (3)	0.001 (2)	−0.006 (2)
C2	0.048 (3)	0.044 (3)	0.039 (3)	0.000 (3)	0.000 (2)	0.002 (2)
C3	0.042 (3)	0.037 (3)	0.044 (3)	0.002 (2)	0.011 (2)	0.004 (2)

C4	0.061 (4)	0.049 (4)	0.051 (4)	0.000 (3)	−0.017 (3)	0.008 (3)
C5	0.049 (4)	0.062 (3)	0.084 (4)	−0.002 (4)	−0.015 (4)	0.008 (3)
C6	0.051 (4)	0.041 (3)	0.061 (4)	−0.006 (3)	−0.008 (3)	0.005 (3)
C7	0.055 (4)	0.043 (4)	0.040 (3)	0.008 (3)	0.006 (3)	−0.008 (3)
C8	0.047 (3)	0.032 (3)	0.040 (3)	−0.003 (3)	0.007 (3)	−0.001 (3)
C9	0.043 (3)	0.047 (4)	0.051 (4)	−0.003 (3)	0.011 (3)	0.003 (3)
C10	0.046 (3)	0.051 (4)	0.045 (3)	0.000 (3)	0.009 (2)	0.004 (3)
C11	0.041 (3)	0.036 (3)	0.041 (2)	0.000 (3)	−0.002 (2)	−0.0006 (17)
C12	0.040 (3)	0.042 (3)	0.046 (3)	0.001 (2)	0.008 (3)	−0.002 (3)
C13	0.046 (4)	0.032 (3)	0.037 (3)	−0.006 (2)	0.007 (2)	−0.002 (2)
C14	0.063 (4)	0.056 (4)	0.061 (4)	0.010 (3)	−0.007 (3)	0.013 (3)
C15	0.108 (7)	0.089 (6)	0.098 (7)	0.025 (5)	0.021 (5)	−0.012 (5)
C16	0.064 (4)	0.061 (3)	0.054 (3)	−0.001 (5)	0.002 (4)	0.018 (2)
C17	0.072 (5)	0.069 (5)	0.114 (6)	−0.019 (4)	0.003 (5)	0.024 (5)
I1	0.0585 (2)	0.05387 (18)	0.05074 (17)	−0.0006 (2)	0.0024 (2)	0.01511 (17)
N1	0.054 (3)	0.036 (2)	0.039 (2)	−0.001 (2)	0.004 (2)	0.003 (2)
N2	0.050 (3)	0.052 (3)	0.041 (2)	0.003 (2)	0.005 (2)	0.011 (2)
O1	0.051 (3)	0.060 (3)	0.048 (3)	0.008 (2)	0.015 (2)	0.013 (2)

Geometric parameters (Å, º)

C1—C2	1.388 (7)	C11—N2	1.381 (7)
C1—C6	1.390 (8)	C11—C12	1.393 (7)
C1—N1	1.407 (7)	C12—C13	1.374 (7)
C2—C3	1.365 (7)	C12—H12	0.9300
C2—H2	0.9300	C13—O1	1.349 (6)
C3—C4	1.381 (8)	C14—N2	1.450 (8)
C3—I1	2.114 (5)	C14—C15	1.503 (10)
C4—C5	1.373 (8)	C14—H14A	0.9700
C4—H4	0.9300	C14—H14B	0.9700
C5—C6	1.384 (8)	C15—H15A	0.9600
C5—H5	0.9300	C15—H15B	0.9600
C6—H6	0.9300	C15—H15C	0.9600
C7—N1	1.292 (7)	C16—N2	1.449 (7)
C7—C8	1.446 (8)	C16—C17	1.512 (9)
C7—H7	0.9300	C16—H16A	0.9700
C8—C9	1.404 (8)	C16—H16B	0.9700
C8—C13	1.409 (8)	C17—H17A	0.9600
C9—C10	1.354 (8)	C17—H17B	0.9600
C9—H9	0.9300	C17—H17C	0.9600
C10—C11	1.430 (9)	O1—H1	0.8200
C10—H10	0.9300		
C2—C1—C6	118.8 (5)	C13—C12—H12	118.7
C2—C1—N1	116.7 (5)	C11—C12—H12	118.7
C6—C1—N1	124.3 (5)	O1—C13—C12	118.7 (5)
C3—C2—C1	120.1 (5)	O1—C13—C8	121.0 (6)
C3—C2—H2	119.9	C12—C13—C8	120.2 (5)
C1—C2—H2	119.9	N2—C14—C15	114.7 (6)
C2—C3—C4	122.0 (5)	N2—C14—H14A	108.6

C2—C3—I1	118.2 (4)	C15—C14—H14A	108.6
C4—C3—I1	119.8 (4)	N2—C14—H14B	108.6
C5—C4—C3	117.6 (5)	C15—C14—H14B	108.6
C5—C4—H4	121.2	H14A—C14—H14B	107.6
C3—C4—H4	121.2	C14—C15—H15A	109.5
C4—C5—C6	121.9 (6)	C14—C15—H15B	109.5
C4—C5—H5	119.0	H15A—C15—H15B	109.5
C6—C5—H5	119.0	C14—C15—H15C	109.5
C5—C6—C1	119.5 (6)	H15A—C15—H15C	109.5
C5—C6—H6	120.3	H15B—C15—H15C	109.5
C1—C6—H6	120.3	N2—C16—C17	114.0 (5)
N1—C7—C8	120.3 (6)	N2—C16—H16A	108.8
N1—C7—H7	119.8	C17—C16—H16A	108.8
C8—C7—H7	119.8	N2—C16—H16B	108.8
C9—C8—C13	117.3 (6)	C17—C16—H16B	108.8
C9—C8—C7	120.6 (5)	H16A—C16—H16B	107.6
C13—C8—C7	122.0 (6)	C16—C17—H17A	109.5
C10—C9—C8	122.5 (6)	C16—C17—H17B	109.5
C10—C9—H9	118.8	H17A—C17—H17B	109.5
C8—C9—H9	118.8	C16—C17—H17C	109.5
C9—C10—C11	120.6 (5)	H17A—C17—H17C	109.5
C9—C10—H10	119.7	H17B—C17—H17C	109.5
C11—C10—H10	119.7	C7—N1—C1	121.0 (5)
N2—C11—C12	122.1 (5)	C11—N2—C16	121.0 (5)
N2—C11—C10	121.2 (4)	C11—N2—C14	120.2 (5)
C12—C11—C10	116.7 (5)	C16—N2—C14	118.6 (5)
C13—C12—C11	122.6 (5)	C13—O1—H1	109.5

C6—C1—C2—C3	1.1 (8)	C10—C11—C12—C13	0.2 (8)
N1—C1—C2—C3	176.8 (5)	C11—C12—C13—O1	179.6 (5)
C1—C2—C3—C4	−1.7 (8)	C11—C12—C13—C8	−1.9 (9)
C1—C2—C3—I1	−179.9 (4)	C9—C8—C13—O1	−178.9 (5)
C2—C3—C4—C5	1.5 (9)	C7—C8—C13—O1	2.5 (8)
I1—C3—C4—C5	179.7 (4)	C9—C8—C13—C12	2.7 (8)
C3—C4—C5—C6	−0.8 (9)	C7—C8—C13—C12	−175.9 (5)
C4—C5—C6—C1	0.3 (9)	C8—C7—N1—C1	172.9 (5)
C2—C1—C6—C5	−0.4 (8)	C2—C1—N1—C7	152.9 (5)
N1—C1—C6—C5	−175.8 (5)	C6—C1—N1—C7	−31.6 (8)
N1—C7—C8—C9	−179.0 (6)	C12—C11—N2—C16	177.3 (5)
N1—C7—C8—C13	−0.4 (9)	C10—C11—N2—C16	−2.5 (8)
C13—C8—C9—C10	−1.9 (9)	C12—C11—N2—C14	−8.6 (8)
C7—C8—C9—C10	176.7 (6)	C10—C11—N2—C14	171.6 (5)
C8—C9—C10—C11	0.3 (9)	C17—C16—N2—C11	85.1 (7)
C9—C10—C11—N2	−179.6 (5)	C17—C16—N2—C14	−89.0 (7)
C9—C10—C11—C12	0.6 (7)	C15—C14—N2—C11	−76.5 (8)
N2—C11—C12—C13	−179.5 (5)	C15—C14—N2—C16	97.7 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.82	1.85	2.577 (6)	147