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2-{[(*E*)-2-Hydroxybenzylidene]amino}-1*H*-isoindole-1,3(2*H*)-dione

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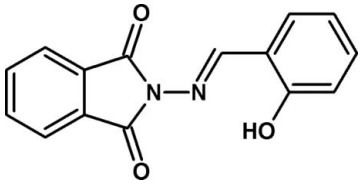
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.098; data-to-parameter ratio = 12.0.

In the title compound, $C_{15}H_{10}N_2O_3$, the isoindoline ring system is almost planar [maximum deviation = 0.020 (2) Å] and makes a dihedral angle of 1.57 (7)° with the benzene ring. Intramolecular O—H···N and C—H···O hydrogen bonds are observed.

Related literature

Based on the multiple binding sites of acetylcholinesterase (AChE), a series of AChE inhibitors involving phthalimide derivatives have been designed and synthesized, see: Zhao *et al.* (2009). Phthalimide derivatives have also been developed as LXRa-selective antagonists, see: Motoshima *et al.* (2009). For the biological activity of Schiff bases, see: Singh *et al.* (2006); Sithambaram *et al.* (2006); Walsh *et al.* (1996). For a related structure, see: Jing *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{10}N_2O_3$
M_r = 266.25
Monoclinic, $P2_1/c$
a = 7.0877 (2) Å
b = 8.2400 (4) Å
c = 21.2752 (7) Å
β = 92.659 (3)°
V = 1241.19 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.22 × 0.15 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.982, T_{max} = 0.988
11806 measured reflections
2184 independent reflections
1541 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.098
S = 1.10
2184 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5···N2	0.82	1.90	2.6152 (16)	145
C9—H9···O4	0.93	2.24	2.8937 (19)	127

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2411).

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2-{[(*E*)-2-Hydroxybenzylidene]amino}-1*H*-isoindole-1,3(2*H*)-dione

H. C. Devarajegowda, H. D. Revanasiddappa, L. Shiva Kumar, V. Sumangala and V. D. Jagadeesh Prasad

S1. Comment

Based on the multiple binding sites of acetylcholinesterase (AChE), a series of AChE inhibitors involving phthalimide derivatives were designed and synthesized (Zhao *et al.,* 2009). Phthalimide derivatives have also been developed as LXRa-selective antagonists (Motoshima *et al.,* 2009). Azomethine group-containing compounds, typically known as Schiff bases, form a significant class of compounds in medicinal and pharmaceutical chemistry, with several biological applications that include antibacterial (Sithambaram Karthikeyan *et al.,* 2006), antifungal (Singh *et al.,* 2006) and antitumor activity (Walsh *et al.,* 1996).

The asymmetric unit of 2-{[(1E)-(2-hydroxyphenyl)methylene]amino} -1*H*-isoindole-1,3(2*H*)-dione contains one molecule (Fig. 1). The isoindoline ring system is almost planar [maximum deviation = 0.020 (2) Å] and makes a dihedral angle of 1.57 (7)° with the benzene ring. The bond distances and bond angles are in good agreement with those in a closely related crystal structure (Jing *et al.,* 2007).

In the crystal structure, molecules intramolecula O5—H5···N2 and C9—H9···O4 hydrogen bonds are observed (Table 1). The packing of the molecules shows stacking when viewed along the *b* axis (Fig. 2).

S2. Experimental

Salicylaldehyde (1.221 g, 10 mmol) was dissolved in 20 ml ethanol and added, with continuous stirring, to a hot ethanolic solution (30 ml) containing *N*-aminophthalimide (1.621 g, 10 mmol). The mixture was further stirred, refluxed for 5 h and allowed to stand overnight. The final yellow product was dissolved in ethanol and a single crystal of the title compound was obtained after slow evaporation of the solvent at room temperature (Yield: 89%; M.p. 465 K).

S3. Refinement

All H atoms were positioned at calculated positions with O—H = 0.82 Å, Csp^2—H = 0.93 Å and refined using a riding model; U_{iso}(H) = kU_{eq}(attached atom), where k = 1.2 for Csp^2 and 1.5 for O.

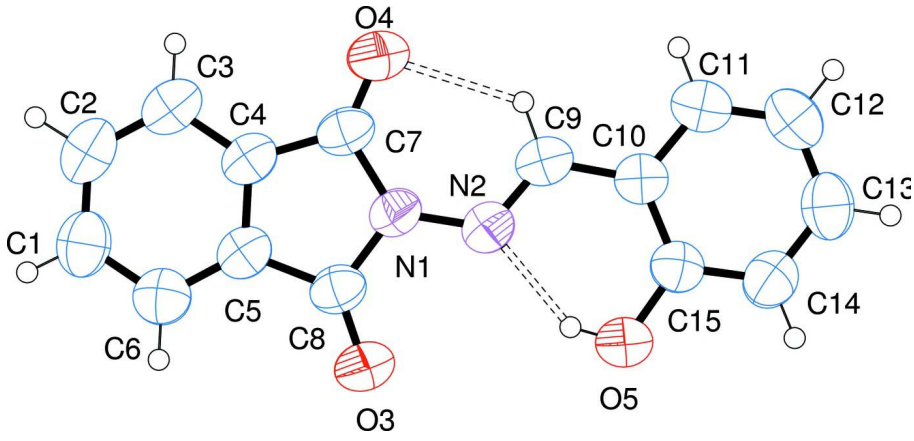

Figure 1

The title molecule with the displacement ellipsoids drawn at the 50% probability level. The H atoms are shown as spheres of arbitrary radius. Dashed lines indicate intramolecular hydrogen bonds.

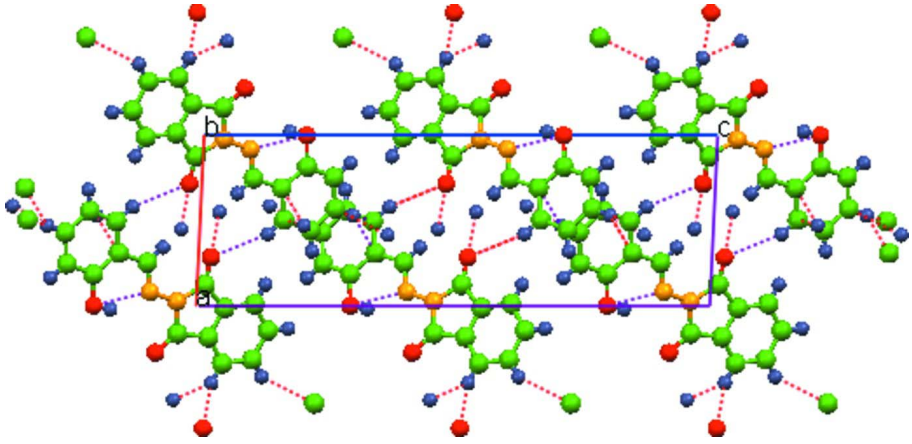

Figure 2

A view of the crystal structure down the *b* axis. Dashed lines indicate intramolecular hydrogen bonds.

2-{[(*E*)-2-Hydroxybenzylidene]amino}-1*H*-isoindole- 1,3(2*H*)-dione

Crystal data

$C_{15}H_{10}N_2O_3$
$M_r = 266.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.0877\ (2)$ Å
$b = 8.2400\ (4)$ Å
$c = 21.2752\ (7)$ Å
$\beta = 92.659\ (3)°$
$V = 1241.19\ (8)$ Å^3
$Z = 4$

$F(000) = 552$
$D_x = 1.425$ Mg m^{-3}
Melting point: 465 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2184 reflections
$\theta = 2.7–25.0°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Plate, yellow
0.22 × 0.15 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.982, T_{max} = 0.988
11806 measured reflections
2184 independent reflections
1541 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.0°, θ_{min} = 2.7°
h = −8→8
k = −9→9
l = −25→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.098
S = 1.10
2184 reflections
182 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0449P)^2 + 0.0801P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0088 (16)

Special details

Experimental. IR ν(Nujolmull, cm^{-1}): 1768 and 1725 (C=O), 1617 (HC=N), 3386 (Ph—OH). ^{1}H NMR (DMSO-d_6, p.p.m.): 10.67 (s, 1H, Ph—OH), 9.45 (s, 1H, HC=N), 6.92–7.91 (m, 4H, Ar—H). FAB-MS: m/z = 267 $[M+1]^+$, Anal. Calc. for $C_{15}H_{10}N_2O_3$; C, 67.67; H, 3.79; N, 10.52; O, 18.03; Found: C, 67.05; H, 3.81; N, 10.68; O, 17.98,; Electronic spectra: 289 nm and 334 nm.

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
O3	−0.27271 (15)	0.27296 (16)	0.07498 (5)	0.0836 (4)
O4	0.28488 (17)	0.31121 (18)	−0.02433 (5)	0.0877 (4)
O5	0.00226 (15)	0.52524 (17)	0.19986 (5)	0.0846 (4)
H5	−0.0194	0.4752	0.1670	0.127*
N1	0.02621 (17)	0.31346 (16)	0.03847 (5)	0.0579 (4)
N2	0.08319 (18)	0.40089 (16)	0.09127 (5)	0.0591 (4)
C1	−0.3130 (3)	0.0248 (2)	−0.11364 (9)	0.0780 (5)
H1	−0.4146	−0.0282	−0.1338	0.094*
C2	−0.1434 (3)	0.0318 (2)	−0.14198 (8)	0.0798 (5)
H2	−0.1320	−0.0162	−0.1812	0.096*
C3	0.0112 (3)	0.1090 (2)	−0.11336 (8)	0.0739 (5)

H3	0.1262	0.1138	−0.1327	0.089*
C4	−0.0109 (2)	0.1786 (2)	−0.05531 (7)	0.0580 (4)
C5	−0.1815 (2)	0.1703 (2)	−0.02662 (7)	0.0578 (4)
C6	−0.3351 (2)	0.0955 (2)	−0.05535 (8)	0.0716 (5)
H6	−0.4506	0.0923	−0.0363	0.086*
C7	0.1244 (2)	0.2722 (2)	−0.01510 (7)	0.0614 (4)
C8	−0.1610 (2)	0.2551 (2)	0.03459 (7)	0.0607 (4)
C9	0.2541 (2)	0.4496 (2)	0.09978 (7)	0.0610 (4)
H9	0.3422	0.4266	0.0700	0.073*
C10	0.3099 (2)	0.54030 (19)	0.15573 (7)	0.0557 (4)
C11	0.4953 (2)	0.5961 (2)	0.16350 (8)	0.0700 (5)
H11	0.5798	0.5748	0.1324	0.084*
C12	0.5558 (3)	0.6816 (2)	0.21590 (9)	0.0783 (5)
H12	0.6801	0.7176	0.2204	0.094*
C13	0.4304 (3)	0.7134 (2)	0.26175 (9)	0.0781 (5)
H13	0.4705	0.7720	0.2973	0.094*
C14	0.2476 (3)	0.6602 (2)	0.25587 (8)	0.0741 (5)
H14	0.1648	0.6823	0.2874	0.089*
C15	0.1854 (2)	0.5737 (2)	0.20321 (8)	0.0610 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0731 (8)	0.1092 (11)	0.0704 (7)	−0.0031 (7)	0.0216 (6)	−0.0101 (7)
O4	0.0713 (8)	0.1189 (12)	0.0746 (8)	−0.0043 (7)	0.0206 (6)	−0.0070 (7)
O5	0.0675 (8)	0.1089 (11)	0.0789 (8)	−0.0129 (7)	0.0191 (6)	−0.0184 (7)
N1	0.0613 (8)	0.0631 (9)	0.0498 (7)	0.0052 (6)	0.0078 (6)	0.0018 (7)
N2	0.0640 (9)	0.0584 (9)	0.0550 (8)	0.0062 (7)	0.0045 (6)	0.0027 (6)
C1	0.0967 (14)	0.0658 (13)	0.0705 (11)	0.0020 (10)	−0.0077 (10)	−0.0015 (10)
C2	0.1067 (15)	0.0726 (14)	0.0597 (10)	0.0146 (11)	0.0006 (10)	−0.0049 (9)
C3	0.0871 (12)	0.0750 (13)	0.0606 (10)	0.0132 (10)	0.0139 (9)	0.0029 (9)
C4	0.0706 (10)	0.0528 (10)	0.0510 (8)	0.0114 (8)	0.0071 (7)	0.0108 (8)
C5	0.0692 (10)	0.0525 (10)	0.0520 (8)	0.0090 (8)	0.0047 (7)	0.0111 (7)
C6	0.0745 (11)	0.0693 (12)	0.0711 (11)	0.0009 (9)	0.0043 (9)	0.0073 (10)
C7	0.0654 (10)	0.0640 (12)	0.0558 (9)	0.0106 (9)	0.0127 (8)	0.0093 (8)
C8	0.0641 (10)	0.0632 (12)	0.0556 (9)	0.0072 (8)	0.0105 (8)	0.0083 (8)
C9	0.0626 (10)	0.0622 (11)	0.0589 (9)	0.0106 (8)	0.0100 (7)	0.0092 (8)
C10	0.0587 (9)	0.0502 (10)	0.0581 (9)	0.0058 (7)	0.0031 (7)	0.0097 (7)
C11	0.0626 (11)	0.0696 (13)	0.0781 (11)	0.0025 (9)	0.0079 (8)	0.0107 (10)
C12	0.0713 (11)	0.0699 (13)	0.0928 (14)	−0.0089 (9)	−0.0062 (10)	0.0072 (11)
C13	0.0924 (14)	0.0607 (13)	0.0797 (12)	−0.0031 (10)	−0.0130 (10)	−0.0018 (10)
C14	0.0827 (12)	0.0714 (13)	0.0687 (11)	0.0012 (10)	0.0076 (9)	−0.0059 (10)
C15	0.0612 (10)	0.0568 (11)	0.0653 (10)	0.0005 (8)	0.0048 (8)	0.0043 (8)

Geometric parameters (Å, º)

O3—C8	1.2041 (17)	C4—C7	1.473 (2)
O4—C7	1.2068 (17)	C5—C6	1.370 (2)

O5—C15	1.3568 (18)	C5—C8	1.479 (2)
O5—H5	0.8200	C6—H6	0.9300
N1—N2	1.3791 (17)	C9—C10	1.445 (2)
N1—C7	1.4044 (19)	C9—H9	0.9300
N1—C8	1.4105 (19)	C10—C11	1.395 (2)
N2—C9	1.2811 (18)	C10—C15	1.399 (2)
C1—C2	1.371 (2)	C11—C12	1.371 (2)
C1—C6	1.386 (2)	C11—H11	0.9300
C1—H1	0.9300	C12—C13	1.375 (2)
C2—C3	1.384 (2)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.368 (2)
C3—C4	1.377 (2)	C13—H13	0.9300
C3—H3	0.9300	C14—C15	1.383 (2)
C4—C5	1.381 (2)	C14—H14	0.9300

C15—O5—H5	109.5	N1—C7—C4	105.31 (13)
N2—N1—C7	130.54 (13)	O3—C8—N1	124.36 (15)
N2—N1—C8	117.71 (11)	O3—C8—C5	130.20 (15)
C7—N1—C8	111.74 (13)	N1—C8—C5	105.43 (12)
C9—N2—N1	121.21 (13)	N2—C9—C10	119.96 (14)
C2—C1—C6	120.94 (17)	N2—C9—H9	120.0
C2—C1—H1	119.5	C10—C9—H9	120.0
C6—C1—H1	119.5	C11—C10—C15	118.16 (15)
C1—C2—C3	121.24 (17)	C11—C10—C9	119.24 (15)
C1—C2—H2	119.4	C15—C10—C9	122.60 (14)
C3—C2—H2	119.4	C12—C11—C10	121.56 (16)
C4—C3—C2	117.71 (16)	C12—C11—H11	119.2
C4—C3—H3	121.1	C10—C11—H11	119.2
C2—C3—H3	121.1	C11—C12—C13	119.14 (17)
C3—C4—C5	120.97 (16)	C11—C12—H12	120.4
C3—C4—C7	129.82 (15)	C13—C12—H12	120.4
C5—C4—C7	109.20 (13)	C14—C13—C12	120.96 (18)
C6—C5—C4	121.26 (15)	C14—C13—H13	119.5
C6—C5—C8	130.43 (14)	C12—C13—H13	119.5
C4—C5—C8	108.30 (14)	C13—C14—C15	120.29 (17)
C5—C6—C1	117.88 (16)	C13—C14—H14	119.9
C5—C6—H6	121.1	C15—C14—H14	119.9
C1—C6—H6	121.1	O5—C15—C14	117.54 (14)
O4—C7—N1	125.03 (16)	O5—C15—C10	122.57 (15)
O4—C7—C4	129.65 (15)	C14—C15—C10	119.88 (15)

C7—N1—N2—C9	−5.3 (2)	C7—N1—C8—O3	178.98 (14)
C8—N1—N2—C9	175.89 (14)	N2—N1—C8—C5	178.99 (12)
C6—C1—C2—C3	0.2 (3)	C7—N1—C8—C5	−0.04 (17)
C1—C2—C3—C4	0.1 (3)	C6—C5—C8—O3	3.4 (3)
C2—C3—C4—C5	0.4 (2)	C4—C5—C8—O3	−177.93 (16)
C2—C3—C4—C7	−177.72 (16)	C6—C5—C8—N1	−177.66 (16)
C3—C4—C5—C6	−1.3 (2)	C4—C5—C8—N1	1.02 (17)

C7—C4—C5—C6	177.25 (15)	N1—N2—C9—C10	−179.69 (13)
C3—C4—C5—C8	179.92 (15)	N2—C9—C10—C11	−178.34 (14)
C7—C4—C5—C8	−1.58 (17)	N2—C9—C10—C15	2.3 (2)
C4—C5—C6—C1	1.5 (2)	C15—C10—C11—C12	−0.1 (2)
C8—C5—C6—C1	−179.97 (16)	C9—C10—C11—C12	−179.50 (15)
C2—C1—C6—C5	−1.0 (3)	C10—C11—C12—C13	−0.2 (3)
N2—N1—C7—O4	−1.0 (3)	C11—C12—C13—C14	0.4 (3)
C8—N1—C7—O4	177.88 (15)	C12—C13—C14—C15	−0.3 (3)
N2—N1—C7—C4	−179.74 (14)	C13—C14—C15—O5	−179.50 (15)
C8—N1—C7—C4	−0.87 (17)	C13—C14—C15—C10	0.0 (3)
C3—C4—C7—O4	1.2 (3)	C11—C10—C15—O5	179.69 (14)
C5—C4—C7—O4	−177.15 (17)	C9—C10—C15—O5	−0.9 (2)
C3—C4—C7—N1	179.85 (16)	C11—C10—C15—C14	0.2 (2)
C5—C4—C7—N1	1.52 (17)	C9—C10—C15—C14	179.56 (15)
N2—N1—C8—O3	−2.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5···N2	0.82	1.90	2.6152 (16)	145
C9—H9···O4	0.93	2.24	2.8937 (19)	127