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(*E*)-2-[(2-Ethylphenyl)iminiomethyl]-6-hydroxyphenolate

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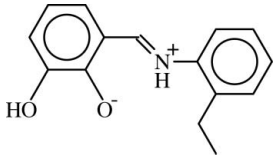
Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.002 Å; R factor = 0.042; wR factor = 0.117; data-to-parameter ratio = 15.9.

The molecule of the title compound, $C_{15}H_{15}NO_2$, crystallizes in a zwitterionic form, and displays an *E* configuration about the C=N bond. The dihedral angle between the two aromatic rings is 5.59 (6)°. An intramolecular N—H···O hydrogen bond generates an $S(6)$ ring motif. In the crystal structure, pairs of molecules are linked into centrosymmetric $R_2^2(10)$ dimers by pairs of O—H···O hydrogen bonds. Aromatic π–π interactions are observed between the benzene rings of adjacent dimers [centroid–centroid distance = 3.4808 (7) Å].

Related literature

For the synthesis, structure and properties of Schiff base complexes, see: Lee *et al.* (2005); Sriram *et al.* (2006); Hao (2009); Bedia *et al.* (2006). For related structures, see: Tüfekçi *et al.* (2009); Yazıcı *et al.* (2010).



Experimental

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Monoclinic, $P2_1/c$
a = 7.7482 (4) Å
b = 10.8713 (7) Å
c = 15.4742 (7) Å
β = 117.380 (3)°
V = 1157.42 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 150 K
0.77 × 0.63 × 0.39 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.945, T_{max} = 0.967
10088 measured reflections
2655 independent reflections
2384 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
S = 1.05
2655 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1	0.92 (2)	1.77 (2)	2.5793 (16)	145 (2)
O2—H2···O1^{i}	0.82	2.13	2.6993 (12)	127

Symmetry code: (i) $-x+2, -y+1, -z+1$.

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* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5022).

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(*E*)-2-[(2-Ethylphenyl)iminiomethyl]-6-hydroxyphenolate

Serap Yazıcı, Çiğdem Albayrak, İsmail Gümrükçüoğlu, İsmet Şenel and Orhan Büyükgüngör

S1. Comment

Schiff bases are one of the most prevalent and important mixed-donor ligand in coordination chemistry (Lee *et al.*, 2005). Recently, the synthesis, structure and properties of Schiff base complexes have stimulated much more interest for their noteworthy contributions in pharmaceutical and medicinal activities (Sriram *et al.*, 2006; Hao, 2009; Bedia *et al.*, 2006).

The molecule of the title compound exists in a zwitterionic form, with a strong intramolecular N1—H1···O1 hydrogen bond (Fig. 1). The molecule adopts an E configuration with respect to the amine C═N bond with a C10—C9—N1—C1 torsion angle of 176.29 (10)°. The dihedral angle between the two benzene rings is 5.59 (6)°. The C15—O1 [1.2885 (14) Å], C9—N1 [1.3122 (15) Å] and C9—C10 [1.4071 (16) Å] bond lengths are consistent with corresponding values reported for related zwitterionic compounds (Tüfekçi *et al.*, 2009; Yazıcı *et al.*, 2010).

The crystal packing is stabilized by intermolecular O—H···O hydrogen bonds (Table 1) which link the molecules to form dimers. In addition, π–π interactions are observed between C1–C6 (at x,y,z) and C10–C15 (at 1-x,1-y,1-z) benzene rings [centroid-to-centroid distance = 3.4808 (7) Å].

S2. Experimental

A mixture of 2,3-dihydroxybenzaldehyde (0.5 g, 3.6 mmol) in ethanol (20 ml) and 2-ethylaniline (0.43 g, 3.6 mmol) in ethanol (20 ml) was stirred for 1 h under reflux. Single crystals suitable for X-ray analysis were obtained from ethanol by slow evaporation (yield 85%, m.p. 406-407 K).

S3. Refinement

Atom H1 was located in a difference map and refined freely. The remaining H atoms were placed in calculated positions and constrained to ride on their parents atoms, with C–H = 0.93-0.97 Å , O–H = 0.82 Å, N–H = 0.92 Å and U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(O,C_{methyl}).

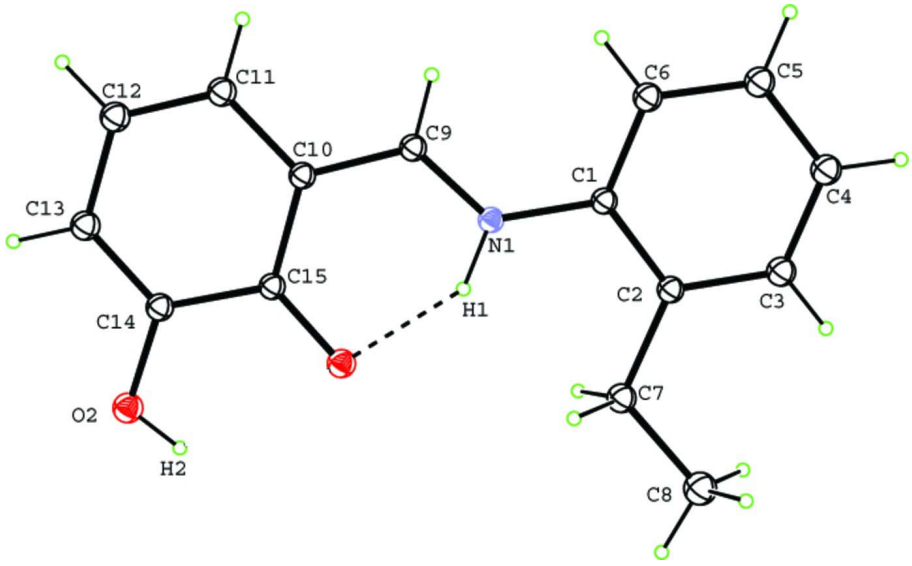

Figure 1

The molecular structure of the title compound, with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

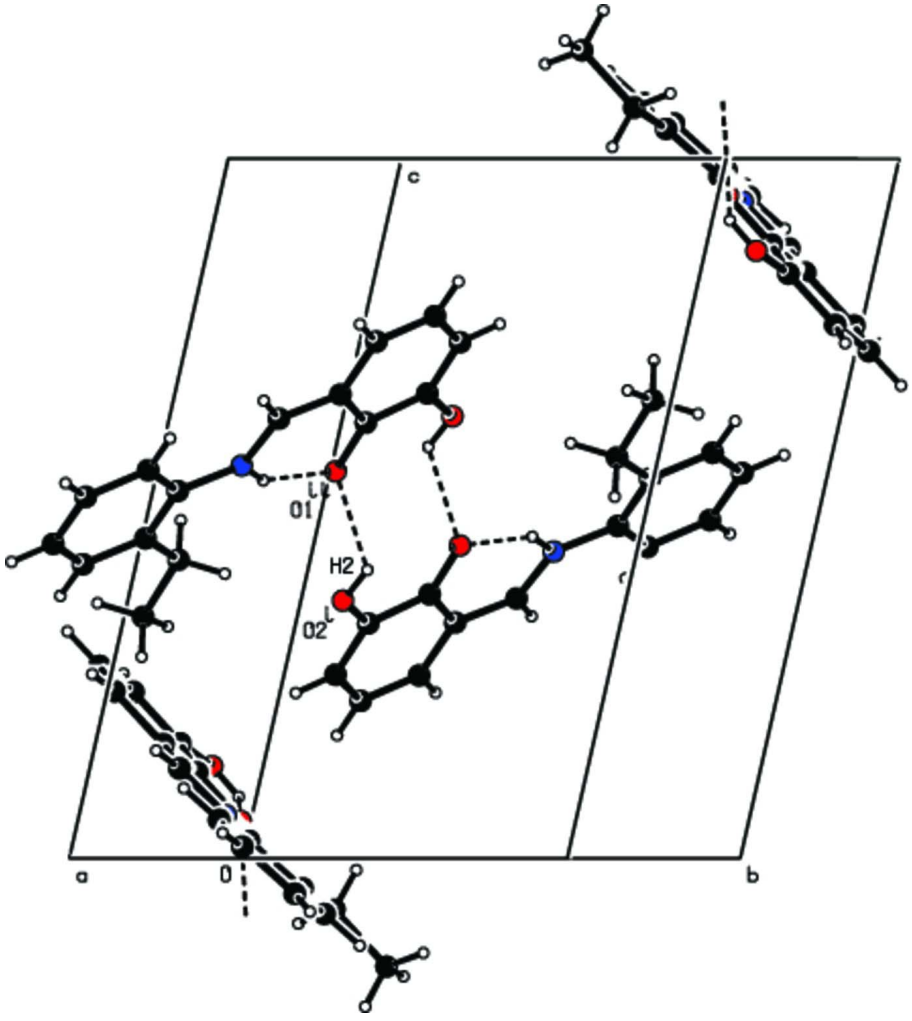

Figure 2

A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines

(*E*)-2-[(2-Ethylphenyl)iminiomethyl]-6-hydroxyphenolate

Crystal data

$C_{15}H_{15}NO_2$
$M_r = 241.28$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.7482\ (4)$ Å
$b = 10.8713\ (7)$ Å
$c = 15.4742\ (7)$ Å
$\beta = 117.380\ (3)°$
$V = 1157.42\ (11)$ Å^3
$Z = 4$

$F(000) = 512$
$D_x = 1.385$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 14793 reflections
$\theta = 2.4–28.0°$
$\mu = 0.09$ mm^{-1}
$T = 150$ K
Prism, red
0.77 × 0.63 × 0.39 mm

Data collection

Stoe IPDS II diffractometer
Radiation source: fine-focus sealed tube

Graphite monochromator
Detector resolution: 6.67 pixels mm^{-1}
ω scan

Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.945, T_{max} = 0.967
10088 measured reflections
2655 independent reflections
2384 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.5°, θ_{min} = 2.4°
h = −10→10
k = −14→14
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.117
S = 1.05
2655 reflections
167 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2 + 0.418P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Special details

Experimental. 196 frames, detector distance = 80 mm The beam size = 0.8 mm.

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
C1	0.36021 (16)	0.72765 (10)	0.47504 (8)	0.0173 (2)
C2	0.48396 (17)	0.81367 (10)	0.54271 (8)	0.0183 (2)
C3	0.40045 (18)	0.89865 (11)	0.57970 (9)	0.0220 (3)
H3	0.4791	0.9567	0.6248	0.026*
C4	0.20240 (18)	0.89846 (11)	0.55063 (9)	0.0240 (3)
H4	0.1497	0.9558	0.5764	0.029*
C5	0.08307 (17)	0.81329 (12)	0.48342 (9)	0.0232 (3)
H5	−0.0498	0.8137	0.4639	0.028*
C6	0.16097 (17)	0.72722 (11)	0.44512 (9)	0.0208 (3)
H6	0.0810	0.6698	0.3999	0.025*
C7	0.69934 (17)	0.81261 (11)	0.57319 (9)	0.0221 (3)
H7A	0.7175	0.8322	0.5168	0.026*
H7B	0.7475	0.7297	0.5933	0.026*
C8	0.82267 (19)	0.90037 (13)	0.65481 (10)	0.0300 (3)
H8A	0.9564	0.8927	0.6687	0.045*
H8B	0.8098	0.8806	0.7120	0.045*
H8C	0.7798	0.9833	0.6353	0.045*
C9	0.35682 (16)	0.55612 (10)	0.37159 (8)	0.0182 (2)

H9	0.2228	0.5478	0.3460	0.022*
C10	0.45648 (16)	0.47823 (10)	0.33700 (8)	0.0179 (2)
C11	0.34923 (17)	0.39280 (11)	0.26133 (9)	0.0206 (3)
H11	0.2151	0.3872	0.2367	0.025*
C12	0.44263 (18)	0.31928 (11)	0.22495 (9)	0.0231 (3)
H12	0.3725	0.2634	0.1757	0.028*
C13	0.64667 (18)	0.32805 (11)	0.26231 (9)	0.0225 (3)
H13	0.7088	0.2782	0.2363	0.027*
C14	0.75465 (17)	0.40778 (11)	0.33558 (8)	0.0195 (2)
C15	0.66399 (16)	0.48648 (10)	0.37727 (8)	0.0176 (2)
N1	0.44559 (14)	0.64003 (9)	0.43849 (7)	0.0171 (2)
O1	0.76679 (12)	0.56081 (8)	0.44695 (6)	0.0214 (2)
O2	0.95018 (12)	0.41463 (8)	0.36831 (7)	0.0246 (2)
H2	0.9964	0.4658	0.4120	0.037*
H1	0.578 (3)	0.6363 (18)	0.4597 (13)	0.042 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0190 (5)	0.0158 (5)	0.0176 (5)	0.0033 (4)	0.0090 (4)	0.0031 (4)
C2	0.0184 (5)	0.0182 (5)	0.0183 (5)	0.0016 (4)	0.0086 (4)	0.0026 (4)
C3	0.0237 (6)	0.0198 (6)	0.0221 (6)	0.0015 (4)	0.0102 (5)	−0.0015 (4)
C4	0.0258 (6)	0.0234 (6)	0.0252 (6)	0.0080 (5)	0.0138 (5)	0.0012 (5)
C5	0.0173 (5)	0.0264 (6)	0.0263 (6)	0.0049 (4)	0.0103 (5)	0.0032 (5)
C6	0.0189 (6)	0.0209 (6)	0.0211 (6)	0.0008 (4)	0.0077 (4)	0.0008 (4)
C7	0.0184 (5)	0.0241 (6)	0.0241 (6)	−0.0003 (4)	0.0102 (5)	−0.0038 (5)
C8	0.0218 (6)	0.0349 (7)	0.0311 (7)	−0.0053 (5)	0.0103 (5)	−0.0099 (6)
C9	0.0166 (5)	0.0177 (5)	0.0178 (5)	0.0004 (4)	0.0058 (4)	0.0028 (4)
C10	0.0193 (5)	0.0158 (5)	0.0165 (5)	0.0008 (4)	0.0066 (4)	0.0016 (4)
C11	0.0190 (5)	0.0193 (5)	0.0192 (6)	−0.0008 (4)	0.0051 (4)	0.0007 (4)
C12	0.0264 (6)	0.0192 (5)	0.0184 (6)	−0.0012 (4)	0.0058 (5)	−0.0031 (4)
C13	0.0271 (6)	0.0198 (5)	0.0201 (6)	0.0045 (4)	0.0105 (5)	−0.0013 (4)
C14	0.0195 (5)	0.0192 (5)	0.0186 (5)	0.0031 (4)	0.0078 (4)	0.0026 (4)
C15	0.0195 (5)	0.0149 (5)	0.0171 (5)	0.0010 (4)	0.0072 (4)	0.0015 (4)
N1	0.0161 (5)	0.0168 (4)	0.0177 (5)	0.0017 (3)	0.0072 (4)	0.0009 (4)
O1	0.0179 (4)	0.0207 (4)	0.0221 (4)	−0.0007 (3)	0.0063 (3)	−0.0054 (3)
O2	0.0190 (4)	0.0297 (5)	0.0238 (4)	0.0026 (3)	0.0087 (3)	−0.0052 (4)

Geometric parameters (Å, º)

C1—C6	1.3929 (16)	C8—H8C	0.96
C1—C2	1.4025 (16)	C9—N1	1.3122 (15)
C1—N1	1.4174 (14)	C9—C10	1.4071 (16)
C2—C3	1.3930 (16)	C9—H9	0.93
C2—C7	1.5112 (16)	C10—C11	1.4245 (16)
C3—C4	1.3864 (17)	C10—C15	1.4352 (15)
C3—H3	0.93	C11—C12	1.3617 (17)
C4—C5	1.3818 (18)	C11—H11	0.93

C4—H4	0.93	C12—C13	1.4149 (17)
C5—C6	1.3857 (17)	C12—H12	0.93
C5—H5	0.93	C13—C14	1.3654 (17)
C6—H6	0.93	C13—H13	0.93
C7—C8	1.5194 (17)	C14—O2	1.3607 (14)
C7—H7A	0.97	C14—C15	1.4346 (16)
C7—H7B	0.97	C15—O1	1.2885 (14)
C8—H8A	0.96	N1—H1	0.924 (18)
C8—H8B	0.96	O2—H2	0.82

C6—C1—C2	121.54 (10)	H8A—C8—H8C	109.5
C6—C1—N1	120.96 (10)	H8B—C8—H8C	109.5
C2—C1—N1	117.50 (10)	N1—C9—C10	122.56 (10)
C3—C2—C1	117.50 (11)	N1—C9—H9	118.7
C3—C2—C7	122.13 (11)	C10—C9—H9	118.7
C1—C2—C7	120.37 (10)	C9—C10—C11	119.36 (10)
C4—C3—C2	121.31 (11)	C9—C10—C15	119.90 (10)
C4—C3—H3	119.3	C11—C10—C15	120.74 (10)
C2—C3—H3	119.3	C12—C11—C10	120.16 (11)
C5—C4—C3	120.19 (11)	C12—C11—H11	119.9
C5—C4—H4	119.9	C10—C11—H11	119.9
C3—C4—H4	119.9	C11—C12—C13	119.87 (11)
C4—C5—C6	120.14 (11)	C11—C12—H12	120.1
C4—C5—H5	119.9	C13—C12—H12	120.1
C6—C5—H5	119.9	C14—C13—C12	121.66 (11)
C5—C6—C1	119.32 (11)	C14—C13—H13	119.2
C5—C6—H6	120.3	C12—C13—H13	119.2
C1—C6—H6	120.3	O2—C14—C13	119.73 (11)
C2—C7—C8	115.90 (10)	O2—C14—C15	119.44 (10)
C2—C7—H7A	108.3	C13—C14—C15	120.81 (11)
C8—C7—H7A	108.3	O1—C15—C14	120.55 (10)
C2—C7—H7B	108.3	O1—C15—C10	122.71 (10)
C8—C7—H7B	108.3	C14—C15—C10	116.74 (10)
H7A—C7—H7B	107.4	C9—N1—C1	127.62 (10)
C7—C8—H8A	109.5	C9—N1—H1	110.1 (12)
C7—C8—H8B	109.5	C1—N1—H1	122.3 (12)
H8A—C8—H8B	109.5	C14—O2—H2	109.5
C7—C8—H8C	109.5		

C6—C1—C2—C3	0.44 (17)	C15—C10—C11—C12	−1.24 (17)
N1—C1—C2—C3	−179.08 (10)	C10—C11—C12—C13	−0.15 (18)
C6—C1—C2—C7	−179.48 (11)	C11—C12—C13—C14	0.92 (19)
N1—C1—C2—C7	0.99 (16)	C12—C13—C14—O2	−178.98 (11)
C1—C2—C3—C4	−0.13 (18)	C12—C13—C14—C15	−0.28 (18)
C7—C2—C3—C4	179.79 (11)	O2—C14—C15—O1	−1.89 (17)
C2—C3—C4—C5	−0.24 (19)	C13—C14—C15—O1	179.41 (11)
C3—C4—C5—C6	0.32 (19)	O2—C14—C15—C10	177.64 (10)
C4—C5—C6—C1	−0.02 (18)	C13—C14—C15—C10	−1.06 (16)

C2—C1—C6—C5	−0.37 (17)	C9—C10—C15—O1	2.05 (17)
N1—C1—C6—C5	179.14 (10)	C11—C10—C15—O1	−178.67 (10)
C3—C2—C7—C8	6.54 (17)	C9—C10—C15—C14	−177.46 (10)
C1—C2—C7—C8	−173.55 (11)	C11—C10—C15—C14	1.81 (16)
N1—C9—C10—C11	−177.37 (10)	C10—C9—N1—C1	176.29 (10)
N1—C9—C10—C15	1.91 (17)	C6—C1—N1—C9	4.29 (18)
C9—C10—C11—C12	178.03 (11)	C2—C1—N1—C9	−176.19 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1	0.92 (2)	1.77 (2)	2.5793 (16)	145 (2)
O2—H2···O1^{i}	0.82	2.13	2.6993 (12)	127

Symmetry code: (i) −*x*+2, −*y*+1, −*z*+1.