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4-[(*E*)-(4-Ethoxyphenyl)iminomethyl]-phenol

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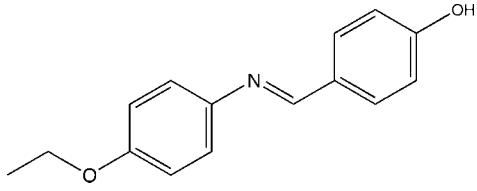
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.031; wR factor = 0.103; data-to-parameter ratio = 11.9.

In the title compound, $C_{15}H_{15}NO_2$, the dihedral angle between the benzene rings is 52.04 (5)° and the molecule has an E conformation about the central C=N bond. In the crystal, molecules are connected by O—H···N hydrogen bonds, forming zigzag chains along the b axis. The crystal packing also features weak C—H···O interactions.

Related literature

For Schiff base derivatives and related structures, see: Fejfarová *et al.* (2010); Özek *et al.* (2010); Akkurt *et al.* (2008); Khalaji *et al.* (2008, 2009) For applications and properties of Schiff bases, see: Dalapati *et al.* (2011); Keypour *et al.* (2010); Khalil *et al.* (2009); Khanmohammadi *et al.* (2009); Sun *et al.* (2012); Da Silva *et al.* (2011).



Experimental

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.3
Orthorhombic, *Pbca*
a = 10.9155 (2) Å
b = 9.4056 (2) Å
c = 25.0422 (5) Å
V = 2571.00 (9) Å^3
Z = 8
Cu $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 120 K
0.54 × 0.20 × 0.03 mm

Data collection

Agilent Xcalibur diffractometer with an Atlas (Gemini ultra Cu) detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
T_{min} = 0.795, T_{max} = 1
22644 measured reflections
1978 independent reflections
1780 reflections with $I > 3\sigma(I)$
R_{int} = 0.028
θ_{max} = 61.1°

Refinement

$R[F^2 > 3\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.103
S = 1.71
1978 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.11 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
C7—H7*b*···O2^{i}	0.96	2.50	3.3393 (15)	147
O2—H2*o*···N1^{ii}	0.894 (17)	1.825 (17)	2.7098 (12)	170.0 (14)

Symmetry codes: (i) $x-\frac{1}{2}, y+1, -z+\frac{3}{2}$; (ii) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2006* (Petříček *et al.*, 2006); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2006*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5991).

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Acta Cryst. (2012). E**68**, o2646 [doi:10.1107/S1600536812034253]

4-[(*E*)-(4-Ethoxyphenyl)iminomethyl]phenol

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S1. Comment

Schiff base compounds exhibit a broad range of biological activities, including antifungal, and antibacterial (Da Silva *et al.*, 2011). They are used as anion sensors (Dalapati *et al.*, 2011; Khalil *et al.*, 2009), non-linear optics compounds (Sun *et al.*, 2012), and as versatile ligands in coordination chemistry (Khanmohammadi *et al.*, 2009; Keypour *et al.*, 2010). The present work is part of a structural study of Schiff bases (Khalaji *et al.*, 2008, 2009; Fejfarová *et al.*, 2010) and we report here the structure of (*E*)-(4-hydroxybenzylidene)-4-ethoxyaniline, (1).

The molecule of (1) (Fig. 1) has an *E* conformation about the central C=N bond and the C=N and C—N bond lengths of 1.2853 (45) and 1.4250 (14) Å agree well with the corresponding distances in other Schiff bases (Akkurt *et al.*, 2008; Özek *et al.*, 2010; Khalaji *et al.*, 2008, 2009; Fejfarová *et al.*, 2010). The dihedral angle between the two benzene rings is 52.04 (5)°. The ethoxy group is almost coplanar with the adjacent ring [dihedral angle 3.51 (12)°]. The molecules are connected by intermolecular O—H···N hydrogen bonds, forming zigzag chains along the *b* axis (Fig. 2). The crystal structure is further stabilized by intermolecular C—H···O hydrogen bonds.

S2. Experimental

To a stirring solution of the 4-hydroxybenzaldehyde (0.2 mmol, in 5 ml of methanol) was added 4-ethoxyaniline (0.2 mmol) in 10 ml of methanol and the mixture was stirred for 1 h in air at 323 K and was then left at room temperature for several days without disturbance yielding suitable crystals of 1 that subsequently were filtered off and washed with Et2O. Yield: 82%.

S3. Refinement

The hydroxyl hydrogen atom was found in difference Fourier maps and its coordinates were refined. All other hydrogen atoms were calculated geometrically and refined as riding on their parent atoms. The methyl H atoms were allowed to rotate freely about the adjacent C–C bond. The displacement coefficients of hydrogen atoms U_{iso}(H) were set to 1.5U_{eq}(C, O) for the methyl- and hydroxyl- groups and to to 1.2U_{eq}(C) for the CH– and CH2- groups.

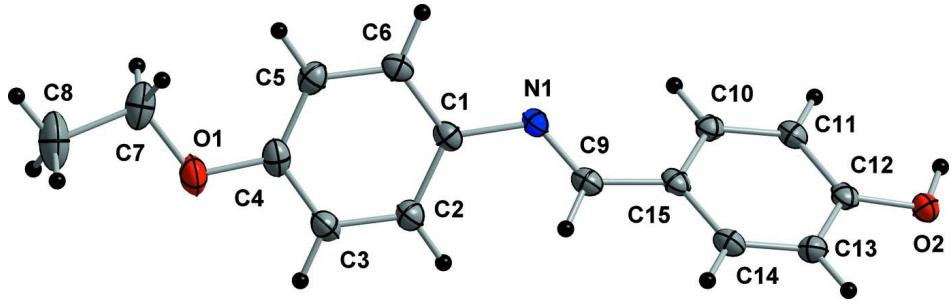

Figure 1

Molecular structure of the title compound. Displacement ellipsoids are shown at the 50% probability level.

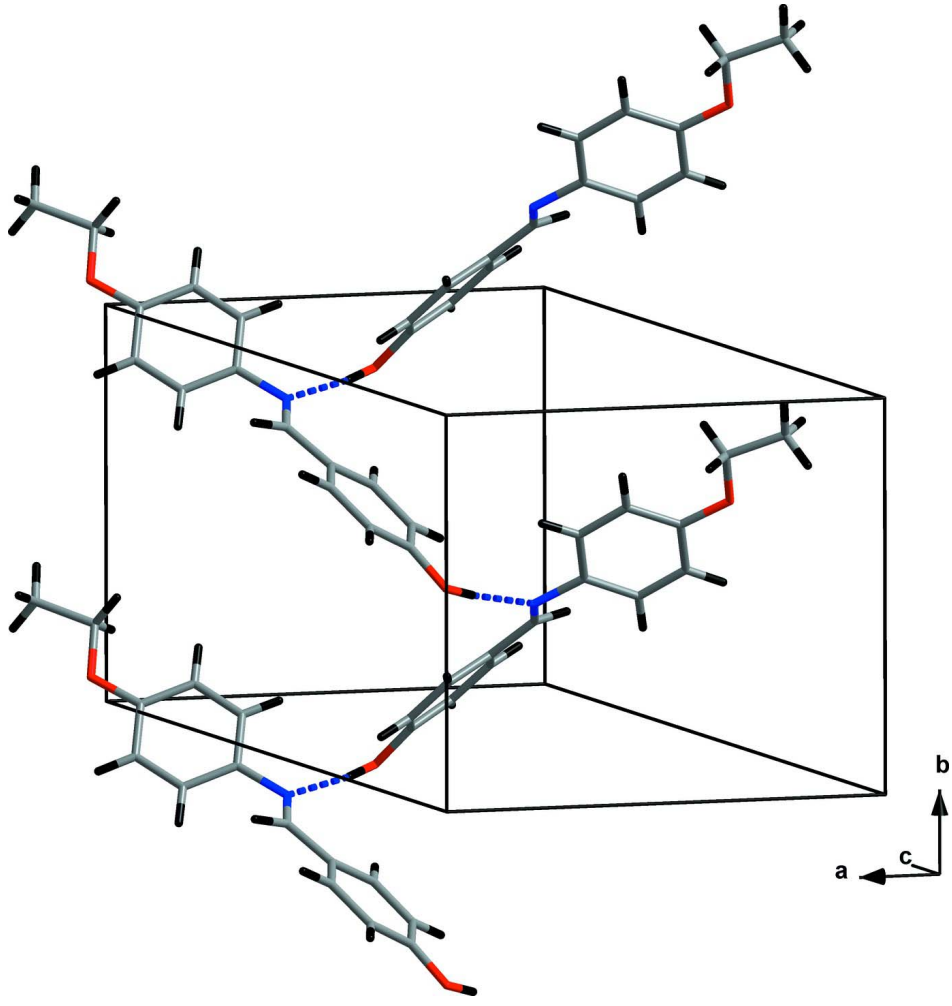

Figure 2

Hydrogen-bonded chain propagating along the *b* axis. Hydrogen bonds are drawn as dashed lines.

4-[(*E*)-(4-Ethoxyphenyl)iminomethyl]phenol

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.3

Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab

a = 10.9155 (2) Å
b = 9.4056 (2) Å
c = 25.0422 (5) Å
V = 2571.00 (9) Å^3
Z = 8
F(000) = 1024
D_x = 1.246 Mg m^{-3}

Cu $K\alpha$ radiation, λ = 1.5418 Å
Cell parameters from 14821 reflections
θ = 3.5–61.1°
μ = 0.67 mm^{-1}
T = 120 K
Plate, light yellow
0.54 × 0.20 × 0.03 mm

Data collection

Agilent Xcalibur diffractometer with an Atlas (Gemini ultra Cu) detector
Radiation source: Enhance Ultra (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.3784 pixels mm^{-1}
Rotation method data acquisition using ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)

T_{min} = 0.795, T_{max} = 1
22644 measured reflections
1978 independent reflections
1780 reflections with $I > 3\sigma(I)$
R_{int} = 0.028
θ_{max} = 61.1°, θ_{min} = 3.5°
h = −12→12
k = −10→10
l = −28→27

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.103
S = 1.71
1978 reflections
166 parameters
0 restraints
57 constraints

H atoms treated by a mixture of independent and constrained refinement
Weighting scheme based on measured s.u.'s $w = 1/(\sigma^2(I) + 0.0025000002I^2)$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.11 e Å^{-3}
$\Delta\rho_{min}$ = −0.11 e Å^{-3}

Special details

Experimental. Absorption correction: CrysAlis PRO (Agilent, 2011). Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

Refinement. The refinement was carried out against all reflections. The conventional *R*-factor is always based on *F*. The goodness of fit as well as the weighted *R*-factor are based on *F* and F^2 for refinement carried out on *F* and F^2, respectively. The threshold expression is used only for calculating *R*-factors *etc*. and it is not relevant to the choice of reflections for refinement.

The program used for refinement, Jana2006, uses the weighting scheme based on the experimental expectations, see _refine_ls_weighting_details, that does not force *S* to be one. Therefore the values of *S* are usually larger than the ones from the *SHELX* program.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.08099 (8)	0.58106 (10)	0.55939 (4)	0.0344 (3)
O2	0.50129 (8)	−0.13939 (9)	0.85269 (3)	0.0251 (3)
N1	0.26997 (8)	0.30259 (10)	0.68326 (4)	0.0196 (3)
C1	0.18053 (10)	0.37189 (12)	0.65100 (4)	0.0200 (3)
C2	0.06035 (11)	0.32217 (13)	0.64660 (4)	0.0234 (4)
C3	−0.02398 (11)	0.39425 (13)	0.61577 (5)	0.0260 (4)
C4	0.00974 (12)	0.51683 (14)	0.58837 (4)	0.0259 (4)
C5	0.12999 (11)	0.56466 (13)	0.59109 (5)	0.0251 (4)
C6	0.21487 (11)	0.49095 (12)	0.62174 (5)	0.0228 (4)

C7	−0.04877 (15)	0.70560 (14)	0.52934 (5)	0.0357 (4)
C8	−0.16378 (16)	0.75963 (18)	0.50327 (7)	0.0509 (5)
C9	0.23493 (11)	0.24457 (11)	0.72715 (5)	0.0208 (4)
C10	0.42099 (10)	0.09397 (12)	0.74119 (5)	0.0198 (4)
C11	0.48630 (10)	−0.00196 (12)	0.77159 (4)	0.0199 (4)
C12	0.44379 (10)	−0.04176 (12)	0.82220 (4)	0.0205 (4)
C13	0.33635 (10)	0.01912 (12)	0.84201 (5)	0.0230 (4)
C14	0.27084 (11)	0.11386 (12)	0.81106 (4)	0.0228 (4)
C15	0.31179 (10)	0.15335 (12)	0.76005 (4)	0.0202 (4)
H2	0.036296	0.23732	0.665154	0.028*
H3	−0.106486	0.35958	0.613196	0.0313*
H5	0.154298	0.648332	0.571861	0.0301*
H6	0.298437	0.52267	0.622731	0.0273*
H7a	0.009871	0.680691	0.502344	0.0429*
H7b	−0.017107	0.776855	0.553066	0.0429*
H8a	−0.144624	0.840538	0.481436	0.0764*
H8b	−0.198521	0.686045	0.48144	0.0764*
H8c	−0.221636	0.786824	0.530273	0.0764*
H9	0.152732	0.262562	0.738996	0.0249*
H10	0.450945	0.120386	0.706538	0.0237*
H11	0.561133	−0.041581	0.758022	0.0239*
H13	0.308026	−0.0049	0.877165	0.0276*
H14	0.196003	0.153391	0.82466	0.0273*
H2o	0.5725 (16)	−0.1625 (16)	0.8374 (6)	0.0377*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0303 (5)	0.0399 (6)	0.0330 (5)	0.0097 (4)	−0.0083 (4)	0.0063 (4)
O2	0.0188 (5)	0.0286 (5)	0.0279 (5)	0.0040 (3)	0.0011 (3)	0.0074 (3)
N1	0.0168 (5)	0.0182 (5)	0.0238 (5)	−0.0005 (4)	−0.0022 (4)	−0.0012 (4)
C1	0.0181 (6)	0.0208 (6)	0.0210 (6)	0.0025 (4)	0.0003 (4)	−0.0033 (5)
C2	0.0218 (6)	0.0235 (7)	0.0248 (6)	−0.0005 (5)	−0.0009 (5)	−0.0002 (5)
C3	0.0180 (6)	0.0325 (7)	0.0277 (7)	0.0002 (5)	−0.0020 (5)	−0.0016 (5)
C4	0.0263 (7)	0.0303 (7)	0.0212 (6)	0.0081 (5)	−0.0028 (5)	−0.0019 (5)
C5	0.0281 (7)	0.0243 (6)	0.0229 (6)	0.0017 (5)	0.0022 (5)	0.0005 (5)
C6	0.0204 (6)	0.0238 (6)	0.0241 (6)	−0.0003 (5)	0.0014 (5)	−0.0020 (5)
C7	0.0496 (9)	0.0313 (7)	0.0262 (7)	0.0121 (6)	−0.0067 (6)	0.0008 (5)
C8	0.0644 (11)	0.0465 (9)	0.0418 (9)	0.0231 (8)	−0.0190 (8)	−0.0003 (7)
C9	0.0166 (6)	0.0199 (6)	0.0259 (7)	−0.0002 (4)	−0.0001 (5)	−0.0030 (5)
C10	0.0176 (6)	0.0207 (6)	0.0209 (6)	−0.0030 (4)	−0.0007 (4)	−0.0011 (4)
C11	0.0154 (6)	0.0205 (6)	0.0239 (6)	−0.0006 (4)	−0.0010 (4)	−0.0023 (5)
C12	0.0169 (6)	0.0196 (6)	0.0249 (6)	−0.0035 (4)	−0.0041 (4)	−0.0005 (5)
C13	0.0190 (6)	0.0271 (7)	0.0228 (6)	−0.0026 (5)	0.0014 (5)	0.0015 (5)
C14	0.0167 (6)	0.0248 (6)	0.0267 (6)	0.0005 (5)	0.0007 (5)	−0.0014 (5)
C15	0.0171 (6)	0.0193 (6)	0.0243 (6)	−0.0030 (4)	−0.0026 (5)	−0.0025 (5)

Geometric parameters (Å, º)

O1—C4	1.3684 (15)	C7—H7a	0.96
O1—C7	1.4360 (16)	C7—H7b	0.96
O2—C12	1.3492 (14)	C8—H8a	0.96
O2—H2o	0.894 (17)	C8—H8b	0.96
N1—C1	1.4250 (14)	C8—H8c	0.96
N1—C9	1.2853 (14)	C9—C15	1.4557 (16)
C1—C2	1.3971 (16)	C9—H9	0.96
C1—C6	1.3897 (16)	C10—C11	1.3791 (16)
C2—C3	1.3795 (17)	C10—C15	1.3985 (15)
C2—H2	0.96	C10—H10	0.96
C3—C4	1.3913 (17)	C11—C12	1.4006 (15)
C3—H3	0.96	C11—H11	0.96
C4—C5	1.3892 (17)	C12—C13	1.3961 (16)
C5—C6	1.3887 (16)	C13—C14	1.3807 (16)
C5—H5	0.96	C13—H13	0.96
C6—H6	0.96	C14—C15	1.4033 (16)
C7—C8	1.504 (2)	C14—H14	0.96
C4—O1—C7	117.43 (10)	C7—C8—H8a	109.47
C12—O2—H2o	109.1 (9)	C7—C8—H8b	109.47
C1—N1—C9	118.37 (9)	C7—C8—H8c	109.47
N1—C1—C2	122.33 (10)	H8a—C8—H8b	109.47
N1—C1—C6	118.86 (10)	H8a—C8—H8c	109.47
C2—C1—C6	118.78 (10)	H8b—C8—H8c	109.47
C1—C2—C3	120.40 (11)	N1—C9—C15	124.24 (10)
C1—C2—H2	119.8	N1—C9—H9	117.88
C3—C2—H2	119.8	C15—C9—H9	117.88
C2—C3—C4	120.45 (11)	C11—C10—C15	121.02 (10)
C2—C3—H3	119.77	C11—C10—H10	119.49
C4—C3—H3	119.77	C15—C10—H10	119.49
O1—C4—C3	115.84 (11)	C10—C11—C12	120.21 (10)
O1—C4—C5	124.54 (11)	C10—C11—H11	119.89
C3—C4—C5	119.61 (11)	C12—C11—H11	119.9
C4—C5—C6	119.73 (11)	O2—C12—C11	122.68 (10)
C4—C5—H5	120.14	O2—C12—C13	117.95 (10)
C6—C5—H5	120.14	C11—C12—C13	119.35 (10)
C1—C6—C5	120.91 (11)	C12—C13—C14	120.02 (11)
C1—C6—H6	119.54	C12—C13—H13	119.99
C5—C6—H6	119.54	C14—C13—H13	119.99
O1—C7—C8	107.38 (12)	C13—C14—C15	121.12 (10)
O1—C7—H7a	109.47	C13—C14—H14	119.44
O1—C7—H7b	109.47	C15—C14—H14	119.44
C8—C7—H7a	109.47	C9—C15—C10	122.37 (10)
C8—C7—H7b	109.47	C9—C15—C14	119.18 (10)
H7a—C7—H7b	111.48	C10—C15—C14	118.24 (10)

C4—O1—C7—C8	−177.51 (11)	N1—C9—C15—C10	−15.04 (18)
C9—N1—C1—C2	−35.10 (15)	N1—C9—C15—C14	170.16 (11)
C9—N1—C1—C6	146.67 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*b*···O2^{i}	0.96	2.50	3.3393 (15)	147
O2—H2*o*···N1^{ii}	0.894 (17)	1.825 (17)	2.7098 (12)	170.0 (14)

Symmetry codes: (i) $x-1/2, y+1, -z+3/2$; (ii) $-x+1, y-1/2, -z+3/2$.