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(*E*)-3-[(2-Fluorophenylimino)methyl]-benzene-1,2-diol

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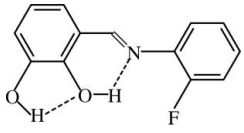
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.040; wR factor = 0.072; data-to-parameter ratio = 15.5.

The title compound, $C_{13}H_{10}FNO_2$, adopts the enol–imine tautomeric form. Intramolecular O—H···O and O—H···N hydrogen bonds generate $S(5)$ and $S(6)$ ring motifs, respectively, whereas intermolecular O—H···O hydrogen bonding links the molecules into centrosymmetric $R_2^2(10)$ dimers. Intermolecular C—H···π and π–π interactions link the molecules into a three-dimensional network. The π–π interactions occur between the fluoro-substituted benzene rings and the centroid-to centroid distance is 3.7590 (12) Å.

Related literature

We have reported the crystal structures of Schiff base systems formed by organic amines and salicylaldehyde derivatives (Temel *et al.*, 2006, 2007*a*,*b*). The title compound, (I), is part of a structural study of these compounds.

For related literature, see: Bernstein *et al.* (1995); Ersanlı *et al.* (2004); Odabaşoğlu *et al.* (2005).



Experimental

Crystal data

$C_{13}H_{10}FNO_2$
M_r = 231.22
Monoclinic, $P2_1/c$
a = 13.6262 (14) Å
b = 6.1497 (4) Å
c = 14.5103 (14) Å
β = 117.307 (7)°
V = 1080.42 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 296 K
0.72 × 0.46 × 0.03 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.940, T_{max} = 0.997
15801 measured reflections
2525 independent reflections
1208 reflections with $I > 2\sigma(I)$
R_{int} = 0.088

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.072
S = 0.80
2525 reflections
163 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C7	1.447 (2)	C7—N1	1.285 (2)
C2—O1	1.3545 (19)	C8—N1	1.412 (2)
N1—C7—C1	120.72 (16)	C7—N1—C8	120.70 (15)
C1—C7—N1—C8	−177.58 (16)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O1^{i}	0.90 (2)	2.11 (2)	2.8474 (18)	138.8 (17)
O2—H2···O1	0.90 (2)	2.209 (19)	2.7237 (17)	116.0 (16)
O1—H1···N1	0.91 (2)	1.74 (2)	2.5637 (18)	150.1 (19)
C6—H6···*Cg*1^{ii}	0.93	2.77	3.519 (2)	138
C10—H10···*Cg*2^{iii}	0.93	2.92	3.615 (2)	133

Symmetry codes: (i) $-x, -y, -z+1$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$. *Cg*1 and *Cg*2 are the centroids of the C1–C6 and C8–C13 rings, respectively.

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).

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS II diffractometer (purchased under grant No. F279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2014).

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supplementary materials

Acta Cryst. (2007). E**63**, o2642 [**doi:10.1107/S1600536807018612**]

(*E*)-3-[(2-Fluorophenylimino)methyl]benzene-1,2-diol

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Comment

We have reported the crystal structures of Schiff base systems formed by organic amines and salicylaldehyde derivatives (Temel *et al.*, 2006; Temel *et al.*, 2007*a*, 2007 b). The title compound, (I), is part of a structural study of these compounds.

Scheme (I)

The compound (I) adopts the enol-imine tautomeric form with an *E* configuration with respect to the C7═N1 double bond, with a C1—C7═N1—C8 torsion angle of 177.58 (16)° and C7═N1—C8 angle of 120.70 (15)° (Fig. 1). The C2—O1 and C7═N1 bond lengths are 1.3545 (19)Å and 1.285 (2) Å, respectively (Table 1), and agree with the corresponding distances in 4-(2-hydroxyphenyliminomethylene)phenol [1.350 (2) Å and 1.285 (2) Å; Ersanlı *et al.*, 2004]. The molecule of (I) is nonplanar, with a dihedral angle between the benzene rings of 52.12 (6)°.

Intra-molecular O—H···O and O—H···N hydrogen bonds generate S(5) and S(6) ring motifs, respectively (Bernstein *et al.*, 1995) (Fig. 1). Molecules of (I) are linked by inter-molecular O—H···O hydrogen bonds, C6—H6···Cg1, C10—H10···Cg2 and Cg2···Cg2 intra-molecular interactions (Cg1 and Cg2 are the centroids of the C1—C6 and C8—C13 rings, respectively) (Fig. 2 and Table 2). The π···π interaction occurs between the C8—C13 ring and its symmetry-related counterpart at (1-x, 1-y, 1-z), with a centroid-to centroid distance of 3.7590 (12) Å and a plane-to-plane separation of 3.467 Å.

Experimental

The title compound was prepared as described by Odabaşoğlu *et al.* (2005), using *o*-bromaniline and 2,3-dihydroxybenzaldehyde as starting materials (yield 75%; m.p. 410-411 K). Crystals of (I) suitable for *X*-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature.

Refinement

The hydroxyl H atoms were located in a difference Fourier synthesis and were refined freely. All H-atoms bound to carbon were refined using a riding model with d(C—H) = 0.93 Å (U_{iso}=1.2U_{eq} of the parent atom) for aromatic and d(C—H) = 0.96 Å (U_{iso}=1.5U_{eq} of the parent atom) for methyl C atoms.

Figures

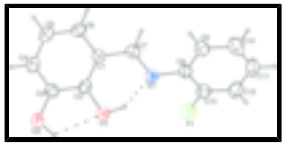

Fig. 1. A view of (I), with the atom numbering scheme and the hydrogen bonds represented as a dashed lines. Thermal ellipsoids are drawn at the 40% probability level.

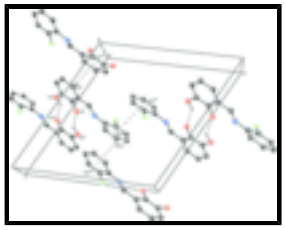

Fig. 2. A packing diagram of (I), showing the intermolecular C—H···π, π-π interactions and O.H···O hydrogen-bonds (dashed lines). H atoms not participating in interaction have been omitted for clarity.

(*E*)-3-[(2-Fluorophenylimino)methyl]benzene-1,2-diol

Crystal data

$C_{13}H_{10}F_1N_1O_2$	F_{000} = 480
M_r = 231.22	D_x = 1.422 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 410-411 K
Hall symbol: -P 2 ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 13.6262 (14) Å	Cell parameters from 10732 reflections
b = 6.1497 (4) Å	θ = 2.8–27.8º
c = 14.5103 (14) Å	μ = 0.11 mm^{-1}
β = 117.307 (7)º	T = 296 K
V = 1080.42 (17) Å^3	Thin plate, brown
Z = 4	0.72 × 0.46 × 0.03 mm

Data collection

Stoe IPDS II diffractometer	2525 independent reflections
Radiation source: fine-focus sealed tube	1208 reflections with $I > 2\sigma(I)$
Monochromator: plane graphite	R_{int} = 0.088
Detector resolution: 6.67 pixels mm^{-1}	θ_{max} = 27.7º
T = 296 K	θ_{min} = 2.8º
ω scans	h = −17→17
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	k = −8→8
T_{min} = 0.940, T_{max} = 0.997	l = −18→18
15801 measured reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0274P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.040	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.072	$\Delta\rho_{max}$ = 0.15 e Å^{-3}
S = 0.80	$\Delta\rho_{min}$ = −0.14 e Å^{-3}

2525 reflections

163 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0054 (7)

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 $F^2 > 2\sigma(F^2)$ 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	0.05535 (13)	0.5384 (3)	0.39129 (13)	0.0344 (4)
C2	0.00883 (13)	0.3482 (3)	0.40674 (12)	0.0360 (4)
C3	−0.10529 (13)	0.3215 (3)	0.35703 (13)	0.0400 (4)
C4	−0.17155 (14)	0.4784 (3)	0.28977 (14)	0.0474 (5)
H4	−0.2477	0.4591	0.2557	0.057*
C5	−0.12565 (14)	0.6651 (3)	0.27237 (14)	0.0492 (5)
H5	−0.1711	0.7692	0.2259	0.059*
C6	−0.01373 (13)	0.6974 (3)	0.32318 (13)	0.0427 (5)
H6	0.0164	0.8247	0.3125	0.051*
C7	0.17369 (14)	0.5714 (3)	0.44446 (13)	0.0393 (4)
H7	0.2031	0.7031	0.4374	0.047*
C8	0.35361 (13)	0.4560 (3)	0.55637 (13)	0.0383 (4)
C9	0.40096 (14)	0.6385 (3)	0.61539 (13)	0.0458 (5)
H9	0.3564	0.7506	0.6178	0.055*
C10	0.51479 (15)	0.6550 (4)	0.67105 (15)	0.0577 (6)
H10	0.5463	0.7784	0.7108	0.069*
C11	0.58167 (15)	0.4898 (4)	0.66797 (16)	0.0588 (6)
H11	0.6580	0.5020	0.7057	0.071*
C12	0.53557 (15)	0.3066 (3)	0.60896 (16)	0.0569 (6)
H12	0.5799	0.1953	0.6054	0.068*
C13	0.42310 (15)	0.2932 (3)	0.55597 (14)	0.0463 (5)
F1	0.37648 (10)	0.11443 (17)	0.49716 (9)	0.0728 (4)
N1	0.23852 (11)	0.4208 (2)	0.50137 (10)	0.0384 (4)
O1	0.07060 (10)	0.18509 (19)	0.46908 (9)	0.0447 (3)
O2	−0.15320 (10)	0.1404 (2)	0.37397 (11)	0.0552 (4)

H1	0.1419 (18)	0.227 (3)	0.4930 (16)	0.081 (7)*
H2	−0.0978 (16)	0.057 (3)	0.4186 (15)	0.069 (7)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0367 (10)	0.0367 (10)	0.0305 (10)	−0.0012 (8)	0.0160 (8)	−0.0015 (8)
C2	0.0352 (9)	0.0390 (10)	0.0308 (9)	0.0041 (8)	0.0124 (8)	−0.0017 (8)
C3	0.0407 (10)	0.0381 (10)	0.0404 (10)	−0.0025 (8)	0.0180 (8)	−0.0029 (9)
C4	0.0373 (10)	0.0543 (12)	0.0433 (11)	0.0045 (9)	0.0123 (9)	0.0003 (10)
C5	0.0478 (12)	0.0513 (12)	0.0435 (11)	0.0147 (9)	0.0168 (9)	0.0101 (9)
C6	0.0477 (11)	0.0403 (10)	0.0410 (10)	0.0044 (8)	0.0210 (9)	0.0066 (9)
C7	0.0464 (11)	0.0388 (10)	0.0370 (10)	−0.0044 (8)	0.0229 (9)	−0.0015 (9)
C8	0.0352 (10)	0.0433 (10)	0.0360 (11)	−0.0011 (8)	0.0160 (9)	0.0037 (9)
C9	0.0444 (11)	0.0478 (11)	0.0453 (11)	−0.0041 (9)	0.0208 (9)	−0.0044 (9)
C10	0.0515 (13)	0.0690 (14)	0.0483 (12)	−0.0165 (11)	0.0191 (10)	−0.0061 (11)
C11	0.0336 (11)	0.0848 (15)	0.0509 (13)	−0.0043 (11)	0.0132 (10)	0.0116 (12)
C12	0.0432 (12)	0.0665 (14)	0.0615 (13)	0.0139 (10)	0.0243 (10)	0.0144 (12)
C13	0.0482 (11)	0.0422 (11)	0.0467 (11)	−0.0012 (9)	0.0203 (9)	0.0022 (9)
F1	0.0696 (8)	0.0509 (7)	0.0902 (9)	0.0049 (6)	0.0299 (7)	−0.0128 (6)
N1	0.0353 (8)	0.0394 (8)	0.0379 (9)	−0.0011 (6)	0.0146 (7)	0.0022 (7)
O1	0.0363 (7)	0.0394 (7)	0.0511 (8)	−0.0001 (6)	0.0136 (6)	0.0091 (6)
O2	0.0340 (7)	0.0486 (8)	0.0703 (10)	−0.0029 (6)	0.0131 (7)	0.0095 (7)

Geometric parameters (Å, °)

C1—C2	1.397 (2)	C8—C9	1.379 (2)
C1—C6	1.402 (2)	C8—C13	1.380 (2)
C1—C7	1.447 (2)	C8—N1	1.412 (2)
C2—O1	1.3545 (19)	C9—C10	1.385 (2)
C2—C3	1.391 (2)	C9—H9	0.9300
C3—O2	1.369 (2)	C10—C11	1.379 (3)
C3—C4	1.375 (2)	C10—H10	0.9300
C4—C5	1.385 (2)	C11—C12	1.380 (3)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.370 (2)	C12—C13	1.366 (3)
C5—H5	0.9300	C12—H12	0.9300
C6—H6	0.9300	C13—F1	1.358 (2)
C7—N1	1.285 (2)	O1—H1	0.91 (2)
C7—H7	0.9300	O2—H2	0.90 (2)
C2—C1—C6	119.33 (15)	C9—C8—C13	117.82 (16)
C2—C1—C7	120.57 (15)	C9—C8—N1	123.87 (16)
C6—C1—C7	120.11 (16)	C13—C8—N1	118.21 (15)
O1—C2—C3	117.57 (15)	C8—C9—C10	120.09 (19)
O1—C2—C1	122.60 (14)	C8—C9—H9	120.0
C3—C2—C1	119.83 (15)	C10—C9—H9	120.0
O2—C3—C4	119.11 (16)	C11—C10—C9	120.46 (19)
O2—C3—C2	120.98 (15)	C11—C10—H10	119.8

C4—C3—C2	119.91 (17)	C9—C10—H10	119.8
C3—C4—C5	120.45 (17)	C10—C11—C12	120.14 (18)
C3—C4—H4	119.8	C10—C11—H11	119.9
C5—C4—H4	119.8	C12—C11—H11	119.9
C6—C5—C4	120.43 (17)	C13—C12—C11	118.19 (19)
C6—C5—H5	119.8	C13—C12—H12	120.9
C4—C5—H5	119.8	C11—C12—H12	120.9
C5—C6—C1	120.00 (18)	F1—C13—C12	118.91 (18)
C5—C6—H6	120.0	F1—C13—C8	117.78 (15)
C1—C6—H6	120.0	C12—C13—C8	123.28 (18)
N1—C7—C1	120.72 (16)	C7—N1—C8	120.70 (15)
N1—C7—H7	119.6	C2—O1—H1	105.9 (14)
C1—C7—H7	119.6	C3—O2—H2	106.4 (13)
C6—C1—C2—O1	178.10 (16)	C6—C1—C7—N1	−175.06 (16)
C7—C1—C2—O1	−1.6 (2)	C13—C8—C9—C10	0.6 (3)
C6—C1—C2—C3	−1.9 (2)	N1—C8—C9—C10	176.77 (17)
C7—C1—C2—C3	178.40 (16)	C8—C9—C10—C11	0.0 (3)
O1—C2—C3—O2	2.5 (2)	C9—C10—C11—C12	0.2 (3)
C1—C2—C3—O2	−177.45 (16)	C10—C11—C12—C13	−1.1 (3)
O1—C2—C3—C4	−177.49 (16)	C11—C12—C13—F1	179.68 (17)
C1—C2—C3—C4	2.5 (3)	C11—C12—C13—C8	1.8 (3)
O2—C3—C4—C5	178.92 (16)	C9—C8—C13—F1	−179.44 (16)
C2—C3—C4—C5	−1.1 (3)	N1—C8—C13—F1	4.1 (2)
C3—C4—C5—C6	−1.0 (3)	C9—C8—C13—C12	−1.5 (3)
C4—C5—C6—C1	1.6 (3)	N1—C8—C13—C12	−177.94 (17)
C2—C1—C6—C5	−0.2 (2)	C1—C7—N1—C8	−177.58 (16)
C7—C1—C6—C5	179.53 (17)	C9—C8—N1—C7	47.3 (2)
C2—C1—C7—N1	4.6 (2)	C13—C8—N1—C7	−136.53 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O1^{i}	0.90 (2)	2.11 (2)	2.8474 (18)	138.8 (17)
O2—H2···O1	0.90 (2)	2.209 (19)	2.7237 (17)	116.0 (16)
O1—H1···N1	0.91 (2)	1.74 (2)	2.5637 (18)	150.1 (19)
C6—H6···Cg1^{ii}	0.93	2.77	3.519 (2)	138
C10—H10···Cg2^{iii}	0.93	2.92	3.615 (2)	133

Symmetry codes: (i) −*x*, −*y*, −*z*+1; (ii) −*x*, *y*+1/2, −*z*+1/2; (iii) −*x*+1, *y*+1/2, −*z*+3/2.

Fig. 1

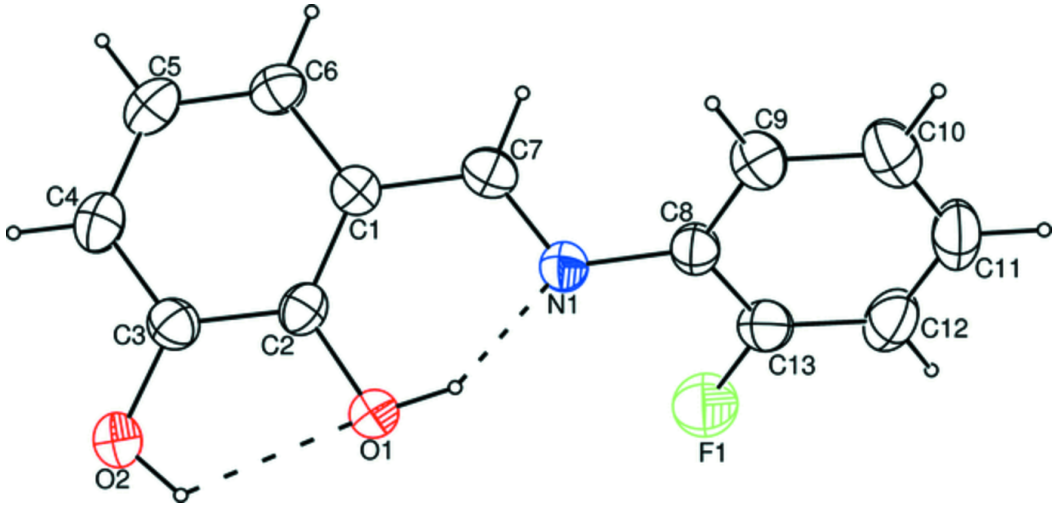

Fig. 2