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# (*E*)-3-[2-(Trifluoromethyl)phenyliminomethyl]-benzene-1,2-diol

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**Key indicators**

Single-crystal X-ray study
*T* = 296 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.060
*wR* factor = 0.169
Data-to-parameter ratio = 14.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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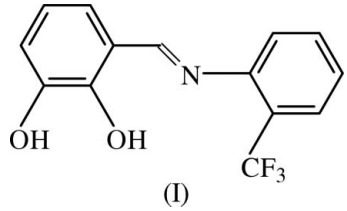
The title compound, $C_{14}H_{10}NO_2F_3$, adopts the enol-imine tautomeric form. There are two independent molecules in the asymmetric unit, with the two aromatic rings inclined at 38.97 (9) and 37.68 (9)°. Each of the independent molecules forms O—H···O hydrogen-bonded centrosymmetric $R_2^2(10)$ dimers.

## Comment

We have reported the crystal structures of Schiff base systems formed by organic amines and salicylaldehyde derivatives (Odabaşoğlu *et al.*, 1999, 2003, 2004, 2005, 2006; Yüce *et al.*, 2004*a*,*b*,*c*, 2006; Şahin *et al.*, 2005*a*,*b*,*c*; Özek *et al.*, 2004*a*,*b*,*c*,*d*, 2005; Albayrak *et al.*, 2005; Koşar *et al.*, 2004, 2005*a*,*b*,*c*; Ersanlı *et al.*, 2003; Ersanlı, Albayrak *et al.*, 2004; Ersanlı, Odabaşoğlu *et al.*, 2004; Temel *et al.*, 2006). The present work is part of a structural study of compounds of Schiff base systems and we report here the structure of the title compound, (I).




(I)

The asymmetric unit of (I) contains two independent molecules, *A* and *B* (Fig. 1). Selected bond lengths and angles are given in Table 1. There is a good agreement between the bond lengths and angles of molecules *A* and *B*. The C2*A*—O1*A*, C7*A*═N1*A*, C2*B*—O1*B* and C7*B*═N1*B* bond lengths confirm the enol-imine form of (I). These distances agree with the corresponding distances in (*E*)-2-methoxy-6-[(2-trifluoromethylphenylimino)methyl]phenol [1.346 (4) Å and 1.270 (5) Å; Şahin *et al.*, 2005*b*], which also adopts the enol-imine form. The dihedral angle between the two benzene rings is 38.97 (9)° in molecule *A* and 37.68 (9)° in molecule *B*.

Intramolecular O—H···N hydrogen bonds are observed in both molecule *A* and *B* (Table 2). Each of these interactions generates an *S*(6) ring motif (Bernstein *et al.*, 1995) [Fig. 1]. In the crystal structure of (I), molecules are linked into *A*—*A* and *B*—*B* type centrosymmetric $R_2^2(10)$ dimers by O—H···O intermolecular hydrogen bonds (Fig. 2).

## Experimental

The title compound was prepared as described by Odabaşoğlu *et al.* (2005), using 2-(trifluoromethyl)aniline and 2,3-dihydroxy-

benzaldehyde as starting materials (yield 73%; m.p. 375–376 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution at room temperature.

*Crystal data*

$C_{14}H_{10}F_3NO_2$
$M_r$ = 281.23
Triclinic, $P\overline{1}$
$a$ = 7.5806 (5) Å
$b$ = 10.5128 (7) Å
$c$ = 16.2370 (11) Å
$\alpha$ = 83.162 (6)°
$\beta$ = 89.612 (6)°
$\gamma$ = 81.938 (6)°
$V$ = 1272.01 (15) Å$^3$
$Z$ = 4
$D_x$ = 1.469 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.13 mm$^{-1}$
$T$ = 296 K
Prismatic needle, red
0.62 × 0.41 × 0.12 mm

*Data collection*

Stoe IPDS-2 diffractometer
$\omega$ scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min}$ = 0.930, $T_{max}$ = 0.985
24664 measured reflections
5534 independent reflections
2951 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.112
$\theta_{max}$ = 27.9°

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.169
$S$ = 1.02
5534 reflections
378 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0768P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.006 (2)

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| C2*A*—O1*A* | 1.359 (3) | C7*B*—N1*B* | 1.286 (3) |
| C2*B*—O1*B* | 1.360 (3) | C8*A*—N1*A* | 1.414 (4) |
| C7*A*—N1*A* | 1.286 (3) | C8*B*—N1*B* | 1.415 (4) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O2*A*—H2*A*···O1*A*$^{i}$ | 0.81 (5) | 2.10 (5) | 2.834 (3) | 149 (5) |
| O2*B*—H2*B*···O1*B*$^{ii}$ | 0.84 (5) | 2.08 (4) | 2.839 (3) | 150 (4) |
| O1*A*—H1*A*···N1*A* | 0.93 (5) | 1.74 (4) | 2.568 (3) | 147 (4) |
| O1*B*—H1*B*···N1*B* | 0.90 (4) | 1.79 (4) | 2.583 (3) | 146 (3) |

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

The crystal was twinned and the reflection data were measured for the two twin domains, scaled and combined together, but overlapping reflections could not be satisfactorily measured and were discarded, leading to a data completeness of only 91%. C-bound H atoms were placed in calculated positions and refined as riding, with C—H = 0.93 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C). The hydroxyl H atoms were located in a difference map and refined freely [O—H = 0.81 (5)–0.93 (5) Å].

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).

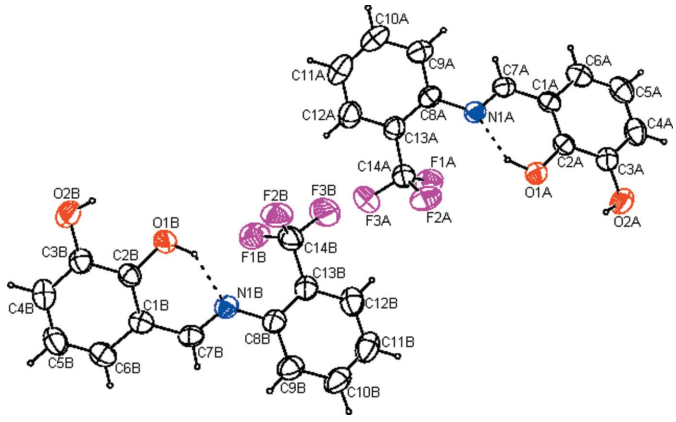



**Figure 1**
The asymmetric unit of (I), showing the atom-numbering scheme and hydrogen bonds as dashed lines. Displacement ellipsoids are drawn at the 40% probability level.

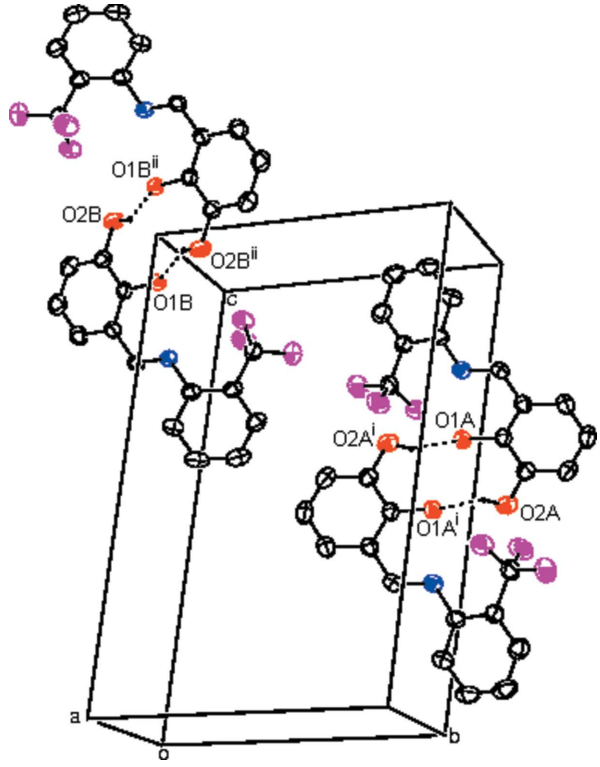



**Figure 2**
A partial packing diagram of (I), showing the $R_2^2(10)$ dimers. Dashed lines indicate hydrogen bonds. H atoms not participating in hydrogen bonding have been omitted for clarity. [Symmetry codes: (i) $1-x, 2-y, 1-z$; (ii) $2-x, -y, 2-z$].

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