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# (*E*)-2-Methoxy-6-[(2-trifluoromethylphenylimino)methyl]phenol

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**Key indicators**

Single-crystal X-ray study
*T* = 296 K
Mean $\sigma$(C–C) = 0.006 Å
*R* factor = 0.054
*wR* factor = 0.123
Data-to-parameter ratio = 8.0

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

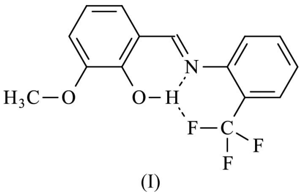
The title compound, $C_{15}H_{12}NO_2F_3$, adopts the phenol–imine tautomeric form. The two aromatic rings are twisted with respect to each other, with a dihedral angle of 17.83 (19)°. O—H···N and O—H···F intramolecular interactions are found in the molecule, and the solid-state structure is stabilized by intermolecular C—H···O and C—H···F hydrogen bonds, to form a two-dimensional network.

## Comment

Much work has been devoted to the physicochemical characterization of substituted aromatic Schiff bases, because these compounds show remarkable photochromic properties, mainly in the solid state (Cohen *et al.*, 1964; Hadjoudis *et al.*, 1987). Photochromism arises from intramolecular H-atom transfer, together with a change in the $\pi$-electron configuration. The effect of intermolecular interactions, such as $\pi$–$\pi$ charge transfer or hydrogen bonding, on H-atom transfer processes has been investigated in the solid state (Hadjoudis *et al.*, 1987; Puranik *et al.*, 1992). *N*-substituted *o*-hydroxyimines have been reported to display photochromism and thermochromism in the solid state by H-atom transfer from the hydroxy O atom to the N atom (Hadjoudis *et al.*, 1987; Xu *et al.*, 1994).

Numerous trifluoromethyl aromatic compounds have higher melting points, sometimes significantly higher, than the corresponding methyl-substituted compounds. Despite their lower molecular weight, trifluoromethyl compounds generally also have higher boiling points. Apparently, stronger forces exist in the crystalline state between molecules containing a $CF_3$ group than in the methyl analogues. These forces do not extend to the liquid state (Boitsov *et al.*, 2002).

*o*-Hydroxyarylidene Schiff bases demonstrate two possible tautomeric forms, keto–amine and phenol–imine. In the solid state, the keto–amine tautomer has been established in naphthaldimine compounds (Hökelek *et al.*, 2000; Ünver *et al.*, 2002) while the phenol–imine tautomer is found in salicylaldimine Schiff bases (Dey *et al.*, 2001; Yang & Vittal, 2003; Karadayı *et al.*, 2003). Against this background, we present here the crystal structure of the title compound, (I).



(I)

Our investigations show that compound (I) adopts the phenol–imine tautomeric form. An *ORTEP3* (Farrugia, 1997)

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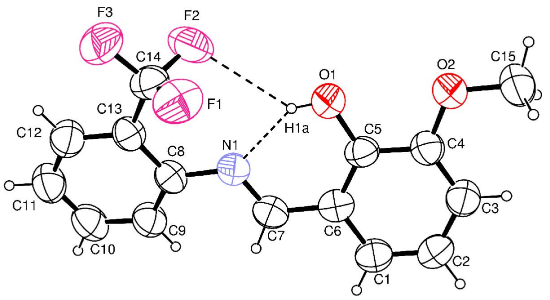

**Figure 1**
A view of the molecule of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed lines indicate hydrogen bonds.

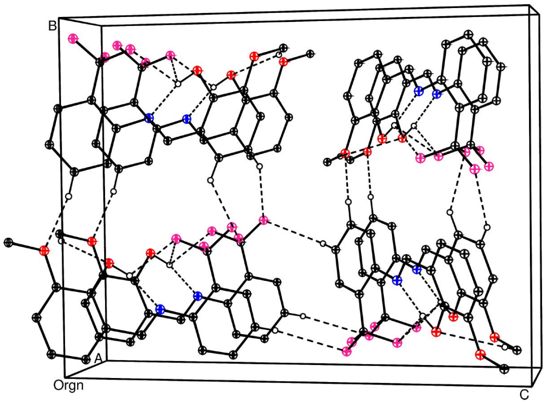

**Figure 2**
A packing diagram for (I). Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

view of the molecule of (I) and a packing diagram are shown in Figs. 1 and 2, respectively. The C8—N1 and C7—C6 bond lengths are 1.418 (5) and 1.454 (5) Å, respectively (Table 1), and agree with the corresponding distances in 2-[(4-hydroxyphenyl)iminomethyl]thiophene [1.422 (2) and 1.447 (3) Å, respectively; Kazak *et al.*, 2000], *trans*-4-[(4-dimethylaminophenyl)iminomethyl]-*N*-methylpyridinium *para*-toluenesulfonate [1.413 (3) and 1.461 Å, respectively; Coe *et al.*, 2001], *N*-[3,5-bis(trifluoromethyl)phenyl]salicylaldimine [1.417 (4) and 1.439 (4) Å, respectively; Karadayı *et al.*, 2003] and *N*-[3,5-bis(trifluoromethyl)phenyl]-3-methoxysalicylaldimine [1.412 (4) and 1.442 (4) Å, respectively; Karadayı *et al.*, 2003]. The N1=C7 bond length of 1.270 (5) Å is typical of a double bond, similar to the corresponding bond lengths in *N*-(2,4-dinitrophenyl)-*N*-methylhydrazone [1.279 (2) Å; Aygün *et al.*, 1998], 2-salicylideneamino-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carbonitrile [1.281 (2) Å; Elerman & Elmalı, 1998] and *N*-[3,5-bis(trifluoromethyl)phenyl]salicylaldimine [1.276 (4) Å; Karadayı *et al.*, 2003]. The O1—C5 and O2—C4 bond lengths are 1.346 (4) and 1.367 (4) Å, respectively, and agree with the corresponding distances in 2-{[tris(hydroxymethyl)methyl]aminomethylene}cyclohexa-3,5-dien-1(2*H*)-one and its 6-hydroxy and 6-methoxy derivatives [1.3025 (16) and 1.3684 (19) Å, respectively; Odabaşoğlu *et al.*, 2003]. The O2—C4 and O2—C15 bond lengths are 1.367 (4) and 1.424 (5) Å, respectively, and these are similar to the corresponding distances in (*E*)-2-hydroxy-3,3′,4′-trimethoxystilbene [1.371 (2) and 1.427 (3) Å, respectively; Stomberg *et al.*, 1998]. The dihedral angle between the C1–C6 and C8–C13 benzene rings is 17.83 (19)°.

Compound (I) forms two strong intramolecular hydrogen bonds [O···N 2.625 (4) Å and O···F 3.199 (4) Å; Table 2], with C5—C6—C7—N1 and C7—C6—C5—O1 torsion angles of −0.6 (5)° and 0.8 (6)°, respectively (Table 1). There are also intermolecular C···F and C···O hydrogen bonds present, producing a two-dimensional network (Fig. 2, Table 2).

## Experimental

The title compound, (I), was prepared by refluxing a solution prepared from *o*-vanillin (0.5 g, 3.286 mmol) in ethanol (10 ml) and 2-(trifloromethyl)aniline (0.529 g, 3.286 mmol) in ethanol (10 ml). The reaction mixture was stirred for 1 h under reflux and left to cool. The product, (I), was recrystallized from methanol (yield 73%; m.p. 390–392 K).

### *Crystal data*

$C_{15}H_{12}F_3NO_2$
$M_r = 295.26$
Orthorhombic, $P2_12_12_1$
$a = 5.2070$ (5) Å
$b = 14.0918$ (18) Å
$c = 18.1737$ (18) Å
$V = 1333.5$ (3) Å$^3$
$Z = 4$
$D_x = 1.471$ Mg m$^{-3}$

Mo *Kα* radiation
Cell parameters from 3996 reflections
$\theta = 1.8$–25.5°
$\mu = 0.13$ mm$^{-1}$
$T = 296$ K
Block, orange
0.50 × 0.29 × 0.18 mm

### *Data collection*

Stoe IPDS 2 diffractometer
$\varphi$ scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.954$, $T_{\max} = 0.979$
8826 measured reflections
1562 independent reflections

931 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.142$
$\theta_{\max} = 26.0°$
$h = -6 \rightarrow 6$
$k = -17 \rightarrow 16$
$l = -22 \rightarrow 22$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.054$
$wR(F^2) = 0.123$
$S = 0.89$
1562 reflections
196 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0641P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.22$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.23$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.015 (3)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—C6 | 1.413 (5) | C6—C7 | 1.454 (5) |
| C3—C4 | 1.370 (5) | C7—N1 | 1.270 (5) |
| C4—O2 | 1.367 (4) | C8—C13 | 1.414 (5) |
| C4—C5 | 1.409 (5) | C8—N1 | 1.418 (5) |
| C5—O1 | 1.346 (4) | C12—C13 | 1.392 (6) |
| C5—C6 | 1.378 (5) | C15—O2 | 1.424 (5) |
| | | | |
| O2—C4—C5 | 114.9 (3) | C13—C8—N1 | 116.7 (3) |
| O1—C5—C6 | 123.1 (4) | C12—C13—C14 | 119.9 (4) |
| C5—C6—C7 | 121.6 (4) | C8—C13—C14 | 121.2 (4) |
| C1—C6—C7 | 118.4 (3) | C7—N1—C8 | 120.5 (3) |
| N1—C7—C6 | 122.0 (3) | C4—O2—C15 | 116.9 (3) |
| C9—C8—N1 | 124.5 (4) | | |
| | | | |
| O1—C5—C6—C7 | 0.8 (6) | C5—C6—C7—N1 | −0.6 (5) |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1$A$···N1 | 1.00 (5) | 1.69 (5) | 2.625 (4) | 154 (4) |
| O1—H1$A$···F2 | 1.00 (5) | 2.57 (5) | 3.199 (4) | 121 (3) |
| C2—H2···F3$^{i}$ | 0.93 | 2.79 | 3.650 (5) | 154 |
| C1—H1···F1$^{i}$ | 0.93 | 2.77 | 3.443 (4) | 130 |
| C10—H10···O2$^{ii}$ | 0.93 | 2.47 | 3.342 (5) | 157 |
| C11—H11···F3$^{iii}$ | 0.93 | 2.90 | 3.751 (5) | 153 |
| C15—H15$B$···O1$^{iv}$ | 0.96 | 2.88 | 3.724 (6) | 148 |

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

The absolute configuration was not determined from the X-ray data, as no strong anomalous scatterer is present; 1069 Friedel pairs were merged before the final refinement. Atom H1*A* bound to O1 was refined freely. All H atoms bound to C atoms were refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic C, and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl C atoms.

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: *ORTEP3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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