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2-Methyl-6-[2-(trifluoromethyl)phenyliminomethyl]phenol

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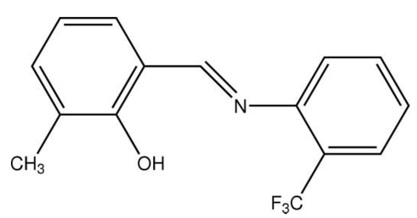
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.081; data-to-parameter ratio = 8.4.

The title compound, $C_{15}H_{12}F_3NO$, is a Schiff base which adopts the phenol–imine tautomeric form in the solid state. The dihedral angle between the aromatic rings is 38.79 (5)°. The molecular structure is stabilized by an intramolecular O—H···N hydrogen bond, which generates an S(6) ring. In addition, there is an intramolecular short C—H···F contact.

Related literature

For the biological properties of Schiff bases, see: Barton *et al.* (1979); Layer (1963); Ingold (1969) Taggi *et al.* (2002); Aydoğan *et al.* (2001). Schiff base compounds can be classified by their photochromic and thermochromic characteristics, see: Cohen *et al.* (1964); Moustakali-Mavridis *et al.* (1978). For the graph-set description of hydrogen bonds, see: Bernstein *et al.* (1995. For a related structure, see: Temel *et al.* (2007).



Experimental

Crystal data

$C_{15}H_{12}F_3NO$
M_r = 279.26
Orthorhombic, $P2_12_12_1$
a = 8.1634 (3) Å
b = 11.8810 (6) Å
c = 13.4469 (7) Å
V = 1304.21 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 K
0.73 × 0.51 × 0.37 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002) T_{min} = 0.943, T_{max} = 0.970
14752 measured reflections
1565 independent reflections
1396 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.081
S = 1.07
1565 reflections
187 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.09 e Å^{-3}
$\Delta\rho_{min}$ = −0.15 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.93 (3)	1.77 (3)	2.619 (2)	151 (3)
C13—H13···F3	0.93	2.36	2.694 (3)	101

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: BT5114).

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supplementary materials

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2-Methyl-6-[2-(trifluoromethyl)phenyliminomethyl]phenol

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Comment

Schiff bases, *i.e.*, compounds having a double C=N bond, are used as starting materials in the synthesis of important drugs, such as antibiotics and antiallergic, antiphlogistic, and antitumor substances (Barton *et al.*, 1979; Layer, 1963; Ingold 1969). On the industrial scale, they have a wide range of applications, such as dyes and pigments (Taggi *et al.*, 2002). Schiff bases have also been employed as ligands for the complexation of metal ions (Aydoğan *et al.*, 2001). There are two characteristic properties of Schiff bases, *viz*. Photochromism and thermochromism (Cohen *et al.*, 1964). In general, Schiff bases display two possible tautomeric forms, the phenol-imine (OH) and the keto-amine (NH) forms. Depending on the tautomers, two types of intramolecular hydrogen bonds are observed in Schiff bases: O—H···N in phenol-imine and N—H···O in keto-amine tautomers.

In the title compound (Fig. 1), the molecular structure is not planar. The dihedral angle between the aromatic ring systems [C1/C6 and C9/C14] is 38.79 (5)°. It is also known that Schiff bases may exhibit thermochromism depending on the planarity or non-planarity, respectively (Moustakali-Mavridis *et al.*, 1978).The O—H and C=N bond lengths confirm the phenol-imine form of the title compound. These distances agree with the corresponding distances in (*E*)-3-[2-(Trifluoromethyl)phenyliminomethyl]-benzene-1,2-diol (Temel *et al.*, 2007), which is related structure. The imine group is coplanar with the C1—C6 aromatic ring system as it can be shown by the C2—C1—C8—N1 torsion angle is 1.67 (19)°.

The molecular structure is stabilized by intramolecular hydrogen bonds. An intramolecular O1—H1···N1 hydrogen bond (Fig. 1) generates a six-membered ring, producing an S(6) ring motif (Bernstein *et al.*, 1995), resulting in approximate planarity of the molecular skeleton [O···N= 2.6187 (16) Å]. The crystal structure is further stabilized by intramolecular C—H···F hydrogen bond, namely C13—H13···F3. And also details of the hydrogen bond is shown in Table 1.

Experimental

A solution of 3-methylsalicylaldehyde (0.0233 g, 0.1711 mmol) in ethanol (10 ml) was added to a solution of 2-Triflouromethylaniline (0.0275 g, 0.1711 mmol) in ethanol (20 ml). The reaction mixture was stirred for 2 h underreflux. Single crystals suitable for X-ray analysis were obtained from ethylalcohol by slow evaporation (yield 69%; m.p.408–410 K).

Refinement

C-bound H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2–1.5U_{eq}(C). The position of the H1 atom was obtained from a difference map and this atom was refined freely. Friedel pairs were merged in the final refinement because the value of the absolute structure parameter (Flack, 1983) is meaningless.

Figures

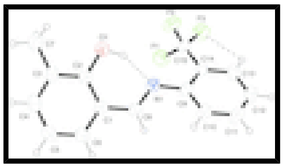

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and 30% probability diplacement ellipsoids.

2-Methyl-6-[2-(trifluoromethyl)phenyliminomethyl]phenol

Crystal data

$C_{15}H_{12}F_3NO$	$F_{000} = 576$
$M_r = 279.26$	$D_x = 1.422$ Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: P 2ac 2ab	Cell parameters from 19471 reflections
$a = 8.1634$ (3) Å	$\theta = 1.5$–28.0°
$b = 11.8810$ (6) Å	$\mu = 0.12$ mm^{-1}
$c = 13.4469$ (7) Å	$T = 293$ K
$V = 1304.21$ (11) Å^3	Prism, light yellow
$Z = 4$	0.73 × 0.51 × 0.37 mm

Data collection

Stoe IPDS II diffractometer	1565 independent reflections
Radiation source: fine-focus sealed tube	1396 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 26.5$°
$T = 293$ K	$\theta_{min} = 2.3$°
rotation method scans	$h = -10 \rightarrow 10$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$k = -14 \rightarrow 14$
$T_{min} = 0.943$, $T_{max} = 0.970$	$l = -16 \rightarrow 16$
14752 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.081$	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.0179P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
1565 reflections	$\Delta\rho_{max} = 0.09$ e Å^{-3}

187 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. 270 frames, detector distance = 100 mm

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.5950 (2)	0.12366 (13)	0.48589 (13)	0.0521 (4)
C2	0.7604 (2)	0.09829 (14)	0.46506 (13)	0.0521 (4)
C3	0.8634 (3)	0.05379 (15)	0.53818 (15)	0.0589 (5)
C4	0.7966 (3)	0.03487 (16)	0.63136 (16)	0.0669 (5)
H4	0.8626	0.0039	0.6806	0.080*
C5	0.6363 (3)	0.06007 (18)	0.65389 (16)	0.0725 (6)
H5	0.5960	0.0471	0.7176	0.087*
C6	0.5366 (3)	0.10426 (16)	0.58227 (15)	0.0653 (5)
H6	0.4285	0.1217	0.5977	0.078*
C7	1.0381 (3)	0.0287 (2)	0.51468 (19)	0.0804 (6)
H7A	1.0972	0.0979	0.5064	0.121*
H7B	1.0440	−0.0144	0.4544	0.121*
H7C	1.0857	−0.0137	0.5682	0.121*
C8	0.4855 (2)	0.16517 (13)	0.41041 (14)	0.0536 (4)
H8	0.3783	0.1826	0.4280	0.064*
C9	0.4144 (2)	0.21161 (13)	0.24725 (14)	0.0525 (4)
C10	0.2558 (3)	0.16864 (15)	0.24564 (17)	0.0638 (5)
H10	0.2227	0.1181	0.2945	0.077*
C11	0.1481 (3)	0.20022 (18)	0.1726 (2)	0.0757 (6)
H11	0.0427	0.1705	0.1720	0.091*
C12	0.1946 (3)	0.27551 (18)	0.10000 (19)	0.0747 (6)
H12	0.1202	0.2976	0.0514	0.090*
C13	0.3510 (3)	0.31792 (17)	0.09962 (16)	0.0661 (5)
H13	0.3827	0.3681	0.0502	0.079*
C14	0.4618 (2)	0.28640 (13)	0.17241 (14)	0.0541 (4)
C15	0.6310 (3)	0.33225 (16)	0.17122 (15)	0.0625 (5)
N1	0.53021 (19)	0.17904 (11)	0.31975 (11)	0.0530 (3)
O1	0.82427 (18)	0.11539 (13)	0.37360 (11)	0.0671 (4)

F1	0.67184 (18)	0.38548 (12)	0.25515 (11)	0.0888 (4)
F2	0.74444 (17)	0.25364 (12)	0.15746 (12)	0.0872 (4)
F3	0.65390 (18)	0.40802 (13)	0.09842 (12)	0.0930 (5)
H1	0.738 (4)	0.141 (2)	0.335 (2)	0.097 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0552 (10)	0.0460 (7)	0.0550 (9)	−0.0031 (7)	0.0000 (8)	−0.0035 (7)
C2	0.0568 (10)	0.0468 (7)	0.0528 (9)	−0.0038 (7)	−0.0010 (8)	−0.0033 (7)
C3	0.0606 (11)	0.0518 (8)	0.0644 (11)	−0.0035 (8)	−0.0118 (9)	−0.0052 (8)
C4	0.0800 (15)	0.0577 (9)	0.0631 (11)	−0.0075 (9)	−0.0180 (11)	0.0033 (8)
C5	0.0891 (16)	0.0757 (11)	0.0528 (11)	−0.0107 (11)	0.0015 (11)	0.0036 (9)
C6	0.0685 (12)	0.0689 (10)	0.0584 (10)	−0.0042 (10)	0.0059 (10)	−0.0013 (9)
C7	0.0621 (13)	0.0903 (14)	0.0889 (16)	0.0081 (11)	−0.0139 (13)	−0.0037 (13)
C8	0.0492 (10)	0.0487 (7)	0.0630 (10)	0.0005 (7)	0.0041 (8)	−0.0018 (7)
C9	0.0490 (9)	0.0471 (7)	0.0613 (10)	0.0058 (7)	−0.0018 (8)	−0.0009 (7)
C10	0.0527 (11)	0.0570 (9)	0.0816 (13)	0.0005 (8)	−0.0025 (10)	0.0039 (10)
C11	0.0528 (11)	0.0695 (11)	0.1048 (17)	0.0025 (9)	−0.0140 (12)	−0.0067 (12)
C12	0.0711 (14)	0.0692 (11)	0.0837 (14)	0.0144 (11)	−0.0227 (12)	−0.0005 (11)
C13	0.0706 (13)	0.0599 (10)	0.0678 (12)	0.0109 (9)	−0.0078 (10)	0.0059 (9)
C14	0.0559 (10)	0.0478 (7)	0.0586 (10)	0.0070 (7)	−0.0011 (8)	−0.0010 (7)
C15	0.0604 (11)	0.0620 (10)	0.0652 (11)	0.0010 (8)	0.0044 (9)	0.0072 (9)
N1	0.0483 (8)	0.0525 (7)	0.0583 (8)	0.0029 (6)	−0.0018 (7)	0.0025 (6)
O1	0.0530 (8)	0.0886 (9)	0.0596 (8)	0.0050 (7)	0.0044 (7)	0.0051 (7)
F1	0.0835 (10)	0.0967 (9)	0.0861 (9)	−0.0323 (8)	0.0002 (8)	−0.0127 (7)
F2	0.0565 (7)	0.0926 (8)	0.1124 (11)	0.0123 (7)	0.0131 (7)	0.0079 (8)
F3	0.0857 (9)	0.0928 (8)	0.1004 (10)	−0.0116 (8)	0.0083 (8)	0.0376 (8)

Geometric parameters (Å, °)

C1—C6	1.400 (3)	C9—C10	1.392 (3)
C1—C2	1.411 (3)	C9—C14	1.397 (2)
C1—C8	1.440 (3)	C9—N1	1.412 (2)
C2—O1	1.351 (2)	C10—C11	1.371 (3)
C2—C3	1.398 (3)	C10—H10	0.9300
C3—C4	1.385 (3)	C11—C12	1.377 (3)
C3—C7	1.491 (3)	C11—H11	0.9300
C4—C5	1.376 (3)	C12—C13	1.373 (3)
C4—H4	0.9300	C12—H12	0.9300
C5—C6	1.366 (3)	C13—C14	1.385 (3)
C5—H5	0.9300	C13—H13	0.9300
C6—H6	0.9300	C14—C15	1.484 (3)
C7—H7A	0.9600	C15—F2	1.328 (2)
C7—H7B	0.9600	C15—F1	1.336 (2)
C7—H7C	0.9600	C15—F3	1.343 (2)
C8—N1	1.283 (2)	O1—H1	0.93 (3)
C8—H8	0.9300		

C6—C1—C2	118.34 (18)	C10—C9—C14	118.66 (18)
C6—C1—C8	119.82 (18)	C10—C9—N1	122.19 (17)
C2—C1—C8	121.82 (16)	C14—C9—N1	119.10 (17)
O1—C2—C3	117.71 (18)	C11—C10—C9	120.5 (2)
O1—C2—C1	121.19 (17)	C11—C10—H10	119.8
C3—C2—C1	121.10 (18)	C9—C10—H10	119.8
C4—C3—C2	117.4 (2)	C10—C11—C12	120.6 (2)
C4—C3—C7	122.4 (2)	C10—C11—H11	119.7
C2—C3—C7	120.1 (2)	C12—C11—H11	119.7
C5—C4—C3	122.6 (2)	C13—C12—C11	119.8 (2)
C5—C4—H4	118.7	C13—C12—H12	120.1
C3—C4—H4	118.7	C11—C12—H12	120.1
C6—C5—C4	119.7 (2)	C12—C13—C14	120.4 (2)
C6—C5—H5	120.2	C12—C13—H13	119.8
C4—C5—H5	120.2	C14—C13—H13	119.8
C5—C6—C1	120.9 (2)	C13—C14—C9	120.02 (19)
C5—C6—H6	119.6	C13—C14—C15	120.06 (17)
C1—C6—H6	119.6	C9—C14—C15	119.91 (16)
C3—C7—H7A	109.5	F2—C15—F1	106.04 (18)
C3—C7—H7B	109.5	F2—C15—F3	105.81 (17)
H7A—C7—H7B	109.5	F1—C15—F3	105.28 (16)
C3—C7—H7C	109.5	F2—C15—C14	113.09 (15)
H7A—C7—H7C	109.5	F1—C15—C14	113.39 (17)
H7B—C7—H7C	109.5	F3—C15—C14	112.55 (17)
N1—C8—C1	122.48 (18)	C8—N1—C9	120.06 (16)
N1—C8—H8	118.8	C2—O1—H1	105.5 (18)
C1—C8—H8	118.8		

C6—C1—C2—O1	−179.82 (16)	C9—C10—C11—C12	−0.5 (3)
C8—C1—C2—O1	2.1 (2)	C10—C11—C12—C13	1.2 (3)
C6—C1—C2—C3	0.7 (2)	C11—C12—C13—C14	−0.7 (3)
C8—C1—C2—C3	−177.39 (15)	C12—C13—C14—C9	−0.4 (3)
O1—C2—C3—C4	−179.06 (16)	C12—C13—C14—C15	179.73 (18)
C1—C2—C3—C4	0.5 (2)	C10—C9—C14—C13	1.1 (2)
O1—C2—C3—C7	1.1 (3)	N1—C9—C14—C13	178.90 (16)
C1—C2—C3—C7	−179.41 (17)	C10—C9—C14—C15	−179.04 (17)
C2—C3—C4—C5	−1.2 (3)	N1—C9—C14—C15	−1.3 (2)
C7—C3—C4—C5	178.6 (2)	C13—C14—C15—F2	−116.15 (19)
C3—C4—C5—C6	0.8 (3)	C9—C14—C15—F2	64.0 (2)
C4—C5—C6—C1	0.4 (3)	C13—C14—C15—F1	123.08 (19)
C2—C1—C6—C5	−1.1 (3)	C9—C14—C15—F1	−56.8 (2)
C8—C1—C6—C5	176.98 (17)	C13—C14—C15—F3	3.7 (3)
C6—C1—C8—N1	−176.38 (16)	C9—C14—C15—F3	−176.13 (16)
C2—C1—C8—N1	1.6 (3)	C1—C8—N1—C9	175.06 (14)
C14—C9—C10—C11	−0.7 (3)	C10—C9—N1—C8	−39.7 (2)
N1—C9—C10—C11	−178.38 (17)	C14—C9—N1—C8	142.65 (17)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O1—H1···N1	0.93 (3)	1.77 (3)	2.619 (2)	151 (3)
C13—H13···F3	0.93	2.36	2.694 (3)	101

Fig. 1