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(*E*)-4-Fluoro-2-[(phenylimino)methyl]phenol

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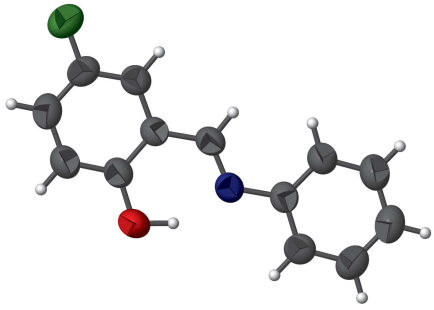
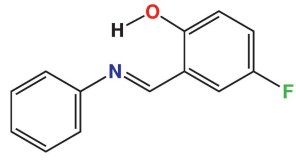
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{13}H_{10}FNO$, is essentially planar (r.m.s. deviation = 0.022 Å) and the dihedral angle between the planes of the two aryl rings is 0.69 (15)°. An intramolecular O—H···N hydrogen bond generates an *S*(6) ring. The crystal structure features C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

We report here, as part of our ongoing research (Ida Malarselvi *et al.*, 2016), the synthesis and crystal structure (Fig. 1), of the title fluorinated Schiff base compound, synthesized from the condensation reaction of equimolar amounts of 5-fluorosalicylaldehyde and aniline in DMSO. In this structure, the benzene and phenyl rings subtend a dihedral angle of 0.69 (15)°. The molecule has an *E* conformation about the C=N bond, and the C1—C7=N1—C8 torsion angle is 180.0 (2)°. There is a strong intramolecular O1—H1···N1 hydrogen bond [H···N = 1.70 (5) Å], which generates an S(6) ring. The crystal structure features C7—H7···O1 hydrogen bonds (see Table 1, Fig. 2).

Yan *et al.*, (2014) have reported the crystal structure of 4-bromo-2-[(phenylimino)-methyl]phenol, in which the molecule is essentially planar (r.m.s. deviation = 0.026 Å), similar to our present study (r.m.s. deviation = 0.022 Å).

Synthesis and crystallization

0.35 g (0.0025 mol) of 5-fluorosalicylaldehyde were dissolved in 10 ml of DMSO. To this solution, 0.23 g (0.0025 mol) of aniline were added drop wise with constant stirring for 1 h. During this time, the solution turned deep yellow. On standing for two weeks with

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O1^{i}	0.93	2.61	3.440 (3)	149
O1—H1···N1	0.99 (4)	1.70 (5)	2.595 (3)	148 (4)

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

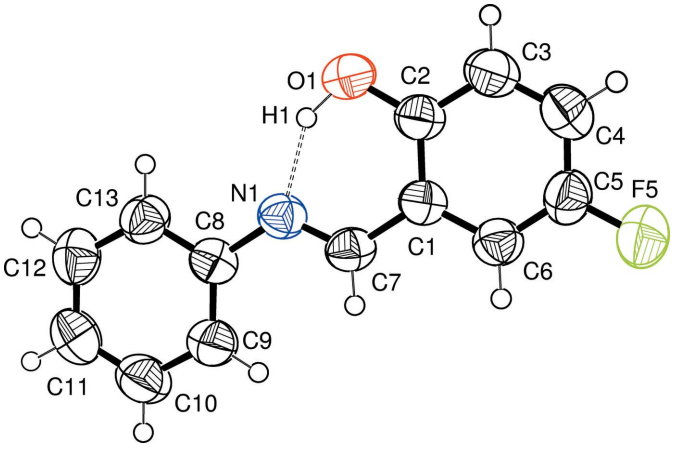


Figure 1
A view of the title compound, with displacement ellipsoids drawn at the 50% probability level. Dashed lines indicate the intramolecular hydrogen bond.

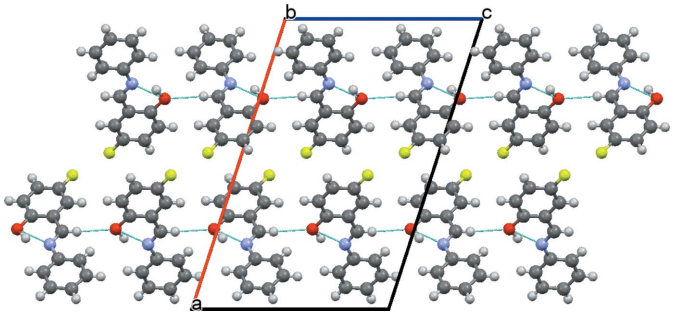


Figure 2
The crystal packing of the title compound, viewed down the crystallographic *b* axis. The hydrogen bonds (see Table 1) are shown as dashed lines.

slow evaporation of the solvent, orange crystals of the title compound, suitable for X-ray study were obtained.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{10}FNO$
M_r	215.22
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	18.965 (2), 4.7214 (5), 12.2399 (13)
β (°)	107.881 (7)
V (Å^3)	1043.0 (2)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.83
Crystal size (mm)	0.30 × 0.20 × 0.10
Data collection	
Diffractometer	Bruker Kappa APEX3CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.536, 0.754
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10586, 1997, 1069
R_{int}	0.097
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.173, 1.03
No. of reflections	1997
No. of parameters	150
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.16

Computer programs: *APEX3*, *SAINT* and *XPREP* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2017* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

Acknowledgements

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References

Bruker (2016). *APEX3*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Ida Malarselvi, R., Ramachandra Raja, C., Thiruvalluvar, A., Priscilla, J. & Panneer Selvam, K. (2016). *IUCrData*, **1**, x161595.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.
Yan, X.-X., Lu, L.-P. & Zhu, M.-L. (2014). *Acta Cryst.* E**70**, o853.

full crystallographic data

IUCrData (2017). **2**, x171671 [https://doi.org/10.1107/S2414314617016716]

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Crystal data

$C_{13}H_{10}FNO$
M_r = 215.22
Monoclinic, $P2_1/c$
a = 18.965 (2) Å
b = 4.7214 (5) Å
c = 12.2399 (13) Å
β = 107.881 (7)°
V = 1043.0 (2) Å^3
Z = 4
$F(000)$ = 448
D_x = 1.371 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 2681 reflections
θ = 4.9–70.9°
μ = 0.83 mm^{-1}
T = 296 K
Plate, orange
0.30 × 0.20 × 0.10 mm

Data collection

Bruker Kappa APEX3 CMOS diffractometer
Radiation source: micro-focus sealed tube
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.536, T_{max} = 0.754
10586 measured reflections
1997 independent reflections
1069 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 71.5°, θ_{min} = 2.5°
h = −23→21
k = −4→5
l = −14→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.173
S = 1.03
1997 reflections
150 parameters
0 restraints
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0689P)^2 + 0.2085P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: SHELXL2017 (Sheldrick, 2015b), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0042 (11)

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. H atoms attached to C of (I) were placed in geometrically idealized positions with Csp^2—H = 0.93 Å. The hydroxy H atom, H1, is located in a difference Fourier map and freely refined.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.31946 (14)	0.1990 (6)	0.8556 (2)	0.0569 (7)
C2	0.32137 (16)	0.1370 (6)	0.9681 (2)	0.0642 (8)
C3	0.37148 (17)	−0.0616 (7)	1.0310 (3)	0.0742 (9)
H3	0.373294	−0.100204	1.106307	0.089*
C4	0.41831 (17)	−0.2017 (7)	0.9837 (3)	0.0752 (9)
H4	0.451482	−0.336124	1.025813	0.090*
C5	0.41512 (16)	−0.1390 (7)	0.8726 (3)	0.0711 (8)
C6	0.36730 (16)	0.0553 (6)	0.8083 (2)	0.0664 (8)
H6	0.366494	0.092055	0.733234	0.080*
C7	0.26800 (16)	0.4054 (6)	0.7872 (2)	0.0612 (7)
H7	0.267062	0.436748	0.711738	0.073*
C8	0.17332 (15)	0.7488 (6)	0.7606 (2)	0.0592 (7)
C9	0.16766 (17)	0.8212 (7)	0.6485 (2)	0.0777 (9)
H9	0.198385	0.735704	0.611808	0.093*
C10	0.11625 (19)	1.0209 (7)	0.5914 (3)	0.0869 (10)
H10	0.112828	1.069505	0.516307	0.104*
C11	0.07008 (17)	1.1487 (7)	0.6439 (3)	0.0806 (9)
H11	0.035174	1.280954	0.604422	0.097*
C12	0.07608 (18)	1.0791 (7)	0.7551 (3)	0.0796 (9)
H12	0.045277	1.164804	0.791596	0.096*
C13	0.12772 (16)	0.8821 (7)	0.8129 (3)	0.0711 (8)
H13	0.131820	0.838381	0.888667	0.085*
N1	0.22382 (12)	0.5460 (5)	0.82746 (17)	0.0611 (6)
O1	0.27583 (12)	0.2678 (5)	1.01816 (17)	0.0817 (7)
F5	0.46145 (10)	−0.2803 (4)	0.82560 (15)	0.0977 (7)
H1	0.245 (2)	0.405 (9)	0.961 (4)	0.142 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0652 (16)	0.0505 (17)	0.0541 (14)	−0.0028 (13)	0.0168 (13)	−0.0012 (12)
C2	0.0727 (18)	0.0631 (19)	0.0565 (15)	0.0010 (15)	0.0195 (14)	0.0033 (14)
C3	0.083 (2)	0.076 (2)	0.0601 (17)	0.0034 (17)	0.0173 (16)	0.0073 (15)
C4	0.078 (2)	0.065 (2)	0.0738 (19)	0.0056 (16)	0.0101 (16)	0.0035 (16)
C5	0.0707 (19)	0.066 (2)	0.0771 (19)	0.0069 (16)	0.0242 (16)	−0.0088 (16)
C6	0.0742 (18)	0.065 (2)	0.0595 (15)	0.0016 (15)	0.0201 (14)	−0.0020 (14)
C7	0.0741 (18)	0.0568 (18)	0.0554 (15)	−0.0031 (14)	0.0238 (14)	0.0010 (13)
C8	0.0658 (16)	0.0495 (17)	0.0594 (15)	−0.0036 (13)	0.0151 (14)	0.0007 (13)
C9	0.090 (2)	0.080 (2)	0.0631 (17)	0.0172 (18)	0.0228 (16)	0.0054 (16)
C10	0.101 (3)	0.084 (3)	0.0687 (19)	0.016 (2)	0.0156 (18)	0.0096 (18)
C11	0.076 (2)	0.068 (2)	0.088 (2)	0.0054 (17)	0.0117 (18)	0.0079 (18)
C12	0.074 (2)	0.070 (2)	0.098 (2)	0.0075 (16)	0.0313 (18)	0.0044 (18)
C13	0.078 (2)	0.067 (2)	0.0732 (18)	0.0026 (16)	0.0313 (16)	0.0048 (15)
N1	0.0709 (15)	0.0551 (15)	0.0573 (13)	0.0004 (11)	0.0195 (11)	0.0024 (10)
O1	0.0998 (16)	0.0907 (17)	0.0631 (12)	0.0191 (13)	0.0374 (12)	0.0105 (11)

F5	0.0988 (13)	0.0962 (15)	0.0989 (13)	0.0253 (11)	0.0317 (11)	−0.0080 (11)

Geometric parameters (Å, º)

C1—C6	1.394 (4)	C8—C13	1.376 (4)
C1—C2	1.397 (4)	C8—C9	1.386 (4)
C1—C7	1.450 (4)	C8—N1	1.422 (3)
C2—O1	1.352 (3)	C9—C10	1.382 (4)
C2—C3	1.388 (4)	C9—H9	0.9300
C3—C4	1.370 (4)	C10—C11	1.375 (4)
C3—H3	0.9300	C10—H10	0.9300
C4—C5	1.375 (4)	C11—C12	1.371 (4)
C4—H4	0.9300	C11—H11	0.9300
C5—C6	1.358 (4)	C12—C13	1.378 (4)
C5—F5	1.364 (3)	C12—H12	0.9300
C6—H6	0.9300	C13—H13	0.9300
C7—N1	1.280 (3)	O1—H1	0.99 (4)
C7—H7	0.9300		
C6—C1—C2	119.0 (3)	C13—C8—C9	118.6 (3)
C6—C1—C7	119.7 (2)	C13—C8—N1	116.7 (2)
C2—C1—C7	121.3 (3)	C9—C8—N1	124.7 (3)
O1—C2—C3	118.8 (2)	C10—C9—C8	119.8 (3)
O1—C2—C1	121.6 (3)	C10—C9—H9	120.1
C3—C2—C1	119.6 (3)	C8—C9—H9	120.1
C4—C3—C2	121.0 (3)	C11—C10—C9	121.0 (3)
C4—C3—H3	119.5	C11—C10—H10	119.5
C2—C3—H3	119.5	C9—C10—H10	119.5
C3—C4—C5	118.4 (3)	C12—C11—C10	119.2 (3)
C3—C4—H4	120.8	C12—C11—H11	120.4
C5—C4—H4	120.8	C10—C11—H11	120.4
C6—C5—F5	119.2 (3)	C11—C12—C13	120.1 (3)
C6—C5—C4	122.5 (3)	C11—C12—H12	120.0
F5—C5—C4	118.3 (3)	C13—C12—H12	120.0
C5—C6—C1	119.4 (3)	C8—C13—C12	121.3 (3)
C5—C6—H6	120.3	C8—C13—H13	119.4
C1—C6—H6	120.3	C12—C13—H13	119.4
N1—C7—C1	122.0 (2)	C7—N1—C8	122.2 (2)
N1—C7—H7	119.0	C2—O1—H1	107 (2)
C1—C7—H7	119.0		
C6—C1—C2—O1	−179.4 (3)	C6—C1—C7—N1	−178.9 (3)
C7—C1—C2—O1	−0.5 (4)	C2—C1—C7—N1	2.2 (4)
C6—C1—C2—C3	1.2 (4)	C13—C8—C9—C10	−0.8 (5)
C7—C1—C2—C3	−179.9 (3)	N1—C8—C9—C10	179.7 (3)
O1—C2—C3—C4	179.4 (3)	C8—C9—C10—C11	−0.3 (5)
C1—C2—C3—C4	−1.2 (4)	C9—C10—C11—C12	0.9 (5)
C2—C3—C4—C5	0.7 (5)	C10—C11—C12—C13	−0.3 (5)

C3—C4—C5—C6	−0.2 (5)	C9—C8—C13—C12	1.5 (4)
C3—C4—C5—F5	−179.5 (3)	N1—C8—C13—C12	−179.1 (3)
F5—C5—C6—C1	179.6 (2)	C11—C12—C13—C8	−0.9 (5)
C4—C5—C6—C1	0.2 (5)	C1—C7—N1—C8	180.0 (2)
C2—C1—C6—C5	−0.7 (4)	C13—C8—N1—C7	178.8 (3)
C7—C1—C6—C5	−179.7 (3)	C9—C8—N1—C7	−1.8 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O1^{i}	0.93	2.61	3.440 (3)	149
O1—H1···N1	0.99 (4)	1.70 (5)	2.595 (3)	148 (4)

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