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4-Fluoro-2-[(*E*)-2-pyridyliminomethyl]-phenol

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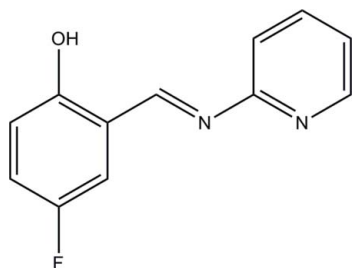
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.053; wR factor = 0.145; data-to-parameter ratio = 12.4.

In the title compound, $\text{C}_{12}\text{H}_9\text{FN}_2\text{O}$, the dihedral angle between the benzene ring and the pyridine ring is $4.35(16)^\circ$. The molecular conformation is stabilized by an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond.

Related literature

For a related structure, see: Li *et al.* (2006). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_9\text{FN}_2\text{O}$ $M_r = 216.21$

Monoclinic, $P2_1/n$
 $a = 13.1635(11)$ Å
 $b = 6.2252(6)$ Å
 $c = 13.8235(17)$ Å
 $\beta = 113.33(3)^\circ$
 $V = 1040.1(3)$ Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 293$ K
 $0.40 \times 0.25 \times 0.15$ mm

Data collection

Enraf-Nonius CAD-4
 diffractometer
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.960$, $T_{\max} = 0.985$

1907 measured reflections
 1825 independent reflections
 1210 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.145$
 $S = 1.05$
 1825 reflections

147 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.17$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{O1}-\text{H1}\cdots\text{N1}$	0.82	1.86	2.588 (2)	147

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2968).

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4-Fluoro-2-[(*E*)-2-pyridyliminomethyl]phenol

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S1. Comment

Recently, we have reported the structural characterization of one Schiff base compound derived from the condensation of 5-chloro-salicylaldehyde and primary amines (Li *et al.*, 2006). As an extension of this work, we report here the crystal structure of the title compound, (I). In (I), all bond lengths are within normal ranges (Allen *et al.*, 1987) (Fig. 1). There is an intramolecular O—H···N hydrogen bond in (I). The dihedral angle between the two aromatic rings is 4.35(0.16)°.

S2. Experimental

Pyridin-2-amine (94 mg, 1 mmol) and 5-fluoro-salicylaldehyde (140 mg, 1 mmol) were dissolved in methanol (10 ml) at 323 K. The mixture was stirred for 2 h to give a clear yellow solution. After keeping the solution in air for 7 d by slow evaporation of the solvent, yellow blocks of (I) were formed at the bottom of the vessel, with 80% yield. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator containing anhydrous CaCl₂.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

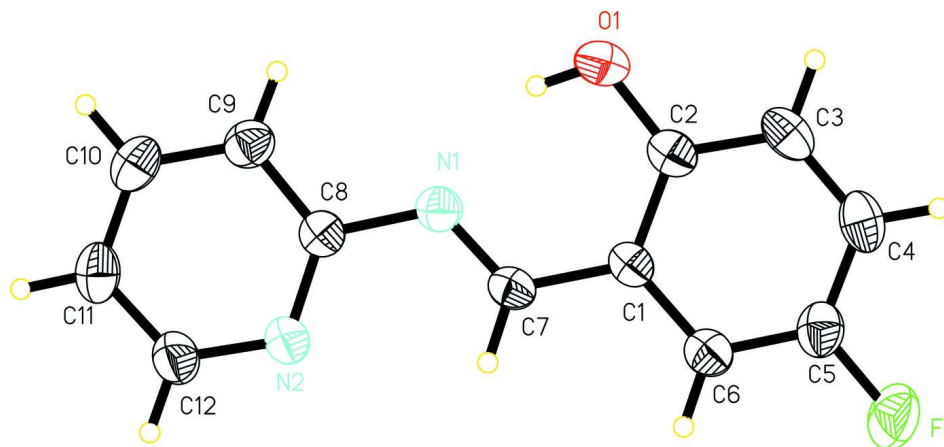


Figure 1

The molecular structure of (I) showing 30% probability displacement ellipsoids.

4-Fluoro-2-[(*E*)-2-pyridyliminomethyl]phenol

Crystal data

C₁₂H₉FN₂O
M_r = 216.21

Monoclinic, *P*2₁/*n*
 Hall symbol: -*P* 2₁*y**n*

$a = 13.1635$ (11) Å
 $b = 6.2252$ (6) Å
 $c = 13.8235$ (17) Å
 $\beta = 113.33$ (3)°
 $V = 1040.1$ (3) Å³
 $Z = 4$
 $F(000) = 448$
 $D_x = 1.381$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 25 reflections
 $\theta = 9\text{--}12^\circ$
 $\mu = 0.10$ mm⁻¹
 $T = 293$ K
 Block, yellow
 $0.40 \times 0.25 \times 0.15$ mm

Data collection

Enraf–Nonius CAD-4
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 $\omega/2\theta$ scans
 Absorption correction: ψ scan
 (North *et al.*, 1968)
 $T_{\min} = 0.960$, $T_{\max} = 0.985$

1907 measured reflections
 1825 independent reflections
 1210 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.064$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 1.8^\circ$
 $h = 0 \rightarrow 15$
 $k = 0 \rightarrow 7$
 $l = -16 \rightarrow 15$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.145$
 $S = 1.05$
 1825 reflections
 147 parameters
 0 restraints
 Primary atom site location: structure-invariant
 direct methods
 Secondary atom site location: difference Fourier
 map

Hydrogen site location: inferred from
 neighbouring sites
 H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0657P)^2 + 0.1652P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.16$ e Å⁻³
 $\Delta\rho_{\min} = -0.17$ e Å⁻³
 Extinction correction: *SHELXL97* (Sheldrick,
 2008), $F_c^* = kF_c[1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$
 Extinction coefficient: 0.089 (10)

Special details

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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.96836 (16)	0.2734 (3)	0.23488 (17)	0.0457 (6)
C2	1.06679 (18)	0.2492 (4)	0.21918 (18)	0.0529 (6)
C3	1.1349 (2)	0.0730 (4)	0.2622 (2)	0.0633 (7)
H3	1.1996	0.0568	0.2510	0.076*
C4	1.1080 (2)	-0.0767 (4)	0.3207 (2)	0.0658 (7)
H4	1.1540	-0.1936	0.3496	0.079*
C5	1.0116 (2)	-0.0506 (4)	0.3357 (2)	0.0619 (7)

C6	0.94233 (19)	0.1189 (3)	0.29492 (19)	0.0548 (6)
H6	0.8779	0.1318	0.3069	0.066*
C7	0.89393 (17)	0.4506 (3)	0.18913 (17)	0.0484 (6)
H7	0.8301	0.4632	0.2022	0.058*
C8	0.83993 (18)	0.7650 (3)	0.08721 (17)	0.0488 (6)
C9	0.8652 (2)	0.9050 (4)	0.02246 (19)	0.0591 (7)
H9	0.9269	0.8816	0.0070	0.071*
C10	0.7981 (2)	1.0788 (4)	-0.01873 (19)	0.0673 (7)
H10	0.8141	1.1762	-0.0618	0.081*
C11	0.7071 (2)	1.1067 (4)	0.0045 (2)	0.0677 (7)
H11	0.6600	1.2231	-0.0223	0.081*
C12	0.6870 (2)	0.9583 (4)	0.0684 (2)	0.0660 (7)
H12	0.6247	0.9772	0.0835	0.079*
F1	0.98419 (14)	-0.2003 (2)	0.39318 (14)	0.0938 (6)
N1	0.91366 (15)	0.5906 (3)	0.13106 (15)	0.0514 (5)
N2	0.75169 (16)	0.7888 (3)	0.11012 (15)	0.0582 (6)
O1	1.09729 (14)	0.3937 (3)	0.16264 (16)	0.0721 (6)
H1	1.0476	0.4818	0.1364	0.108*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0411 (11)	0.0435 (12)	0.0504 (13)	-0.0015 (10)	0.0159 (10)	-0.0095 (10)
C2	0.0488 (13)	0.0527 (13)	0.0569 (14)	-0.0022 (11)	0.0206 (11)	-0.0129 (12)
C3	0.0499 (14)	0.0678 (17)	0.0690 (16)	0.0094 (13)	0.0201 (13)	-0.0160 (14)
C4	0.0655 (17)	0.0503 (15)	0.0676 (17)	0.0120 (13)	0.0116 (13)	-0.0067 (13)
C5	0.0649 (16)	0.0453 (13)	0.0677 (16)	-0.0035 (12)	0.0181 (13)	0.0006 (12)
C6	0.0502 (13)	0.0500 (14)	0.0638 (15)	-0.0036 (11)	0.0221 (11)	-0.0062 (12)
C7	0.0439 (12)	0.0493 (13)	0.0539 (14)	-0.0027 (10)	0.0216 (11)	-0.0089 (11)
C8	0.0513 (13)	0.0479 (13)	0.0462 (13)	-0.0020 (11)	0.0181 (11)	-0.0058 (11)
C9	0.0651 (16)	0.0579 (15)	0.0577 (15)	-0.0051 (12)	0.0280 (13)	-0.0030 (12)
C10	0.0829 (19)	0.0613 (16)	0.0551 (15)	-0.0051 (15)	0.0248 (14)	0.0088 (13)
C11	0.0761 (18)	0.0572 (16)	0.0582 (15)	0.0115 (14)	0.0143 (14)	0.0083 (13)
C12	0.0631 (16)	0.0661 (16)	0.0678 (16)	0.0146 (13)	0.0249 (13)	0.0088 (14)
F1	0.1042 (13)	0.0645 (10)	0.1094 (13)	0.0031 (9)	0.0390 (10)	0.0279 (9)
N1	0.0525 (11)	0.0486 (11)	0.0553 (12)	-0.0021 (9)	0.0237 (9)	-0.0043 (10)
N2	0.0564 (12)	0.0585 (12)	0.0618 (13)	0.0107 (10)	0.0257 (10)	0.0087 (10)
O1	0.0616 (11)	0.0784 (13)	0.0899 (14)	0.0050 (9)	0.0444 (10)	0.0052 (11)

Geometric parameters (Å, °)

C1—C6	1.399 (3)	C7—H7	0.9300
C1—C2	1.404 (3)	C8—N2	1.328 (3)
C1—C7	1.444 (3)	C8—C9	1.381 (3)
C2—O1	1.353 (3)	C8—N1	1.422 (3)
C2—C3	1.392 (3)	C9—C10	1.370 (3)
C3—C4	1.369 (3)	C9—H9	0.9300
C3—H3	0.9300	C10—C11	1.368 (4)

C4—C5	1.375 (3)	C10—H10	0.9300
C4—H4	0.9300	C11—C12	1.375 (3)
C5—C6	1.362 (3)	C11—H11	0.9300
C5—F1	1.363 (3)	C12—N2	1.335 (3)
C6—H6	0.9300	C12—H12	0.9300
C7—N1	1.279 (3)	O1—H1	0.8200
C6—C1—C2	118.4 (2)	C1—C7—H7	119.2
C6—C1—C7	120.12 (19)	N2—C8—C9	122.8 (2)
C2—C1—C7	121.5 (2)	N2—C8—N1	119.8 (2)
O1—C2—C3	118.8 (2)	C9—C8—N1	117.3 (2)
O1—C2—C1	121.4 (2)	C10—C9—C8	119.1 (2)
C3—C2—C1	119.7 (2)	C10—C9—H9	120.4
C4—C3—C2	121.0 (2)	C8—C9—H9	120.4
C4—C3—H3	119.5	C11—C10—C9	118.9 (2)
C2—C3—H3	119.5	C11—C10—H10	120.6
C3—C4—C5	118.6 (2)	C9—C10—H10	120.6
C3—C4—H4	120.7	C10—C11—C12	118.4 (2)
C5—C4—H4	120.7	C10—C11—H11	120.8
C6—C5—F1	118.9 (2)	C12—C11—H11	120.8
C6—C5—C4	122.4 (2)	N2—C12—C11	123.8 (2)
F1—C5—C4	118.8 (2)	N2—C12—H12	118.1
C5—C6—C1	119.8 (2)	C11—C12—H12	118.1
C5—C6—H6	120.1	C7—N1—C8	120.91 (19)
C1—C6—H6	120.1	C8—N2—C12	117.0 (2)
N1—C7—C1	121.6 (2)	C2—O1—H1	109.5
N1—C7—H7	119.2		
C6—C1—C2—O1	-179.5 (2)	C6—C1—C7—N1	-177.70 (19)
C7—C1—C2—O1	1.6 (3)	C2—C1—C7—N1	1.2 (3)
C6—C1—C2—C3	0.7 (3)	N2—C8—C9—C10	1.3 (3)
C7—C1—C2—C3	-178.2 (2)	N1—C8—C9—C10	-178.0 (2)
O1—C2—C3—C4	179.5 (2)	C8—C9—C10—C11	-0.9 (4)
C1—C2—C3—C4	-0.6 (3)	C9—C10—C11—C12	0.0 (4)
C2—C3—C4—C5	0.4 (4)	C10—C11—C12—N2	0.6 (4)
C3—C4—C5—C6	-0.2 (4)	C1—C7—N1—C8	-179.53 (19)
C3—C4—C5—F1	179.5 (2)	N2—C8—N1—C7	2.8 (3)
F1—C5—C6—C1	-179.4 (2)	C9—C8—N1—C7	-177.8 (2)
C4—C5—C6—C1	0.3 (4)	C9—C8—N2—C12	-0.8 (3)
C2—C1—C6—C5	-0.5 (3)	N1—C8—N2—C12	178.5 (2)
C7—C1—C6—C5	178.4 (2)	C11—C12—N2—C8	-0.2 (4)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
O1—H1 \cdots N1	0.82	1.86	2.588 (2)	147