

1-(4-Fluorophenyl)-2-(1*H*-imidazol-1-yl)-ethanol

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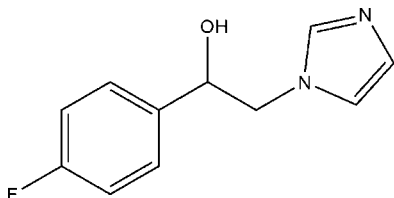
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.041; wR factor = 0.124; data-to-parameter ratio = 7.4.

In the title compound, $\text{C}_{11}\text{H}_{11}\text{FN}_2\text{O}$, the dihedral angle between the mean planes of the two rings is $1.30(4)^\circ$. In the crystal, $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds link the molecules into chains along the b axis.

Related literature

For related compounds containing a 2-(1*H*-imidazol-1-yl)-1-phenylethanol fragment, see: Porretta *et al.* (1993). For related structures, see: Tao *et al.* (2007); Liu *et al.* (2011). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

 $\text{C}_{11}\text{H}_{11}\text{FN}_2\text{O}$
 $M_r = 206.22$

 Monoclinic, $P2_1$
 $a = 7.1220(14)$ Å

 $b = 5.4690(11)$ Å

 $c = 12.981(3)$ Å

 $\beta = 98.13(3)^\circ$
 $V = 500.53(19)$ Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 0.10$ mm⁻¹
 $T = 293$ K

 $0.30 \times 0.20 \times 0.10$ mm

Data collection

Enraf–Nonius CAD-4

diffractometer

Absorption correction: multi-scan

 (North *et al.*, 1968)

 $T_{\min} = 0.970$, $T_{\max} = 0.990$

1992 measured reflections

1024 independent reflections

 876 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

3 standard reflections every 200 reflections

intensity decay: 1%

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.124$
 $S = 1.00$

1024 reflections

139 parameters

1 restraint

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.13$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ e Å⁻³
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O-H\cdots N2^i$	0.87 (4)	1.90 (4)	2.762 (4)	171 (5)

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; 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: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZQ2137).

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supplementary materials

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1-(4-Fluorophenyl)-2-(1*H*-imidazol-1-yl)ethanol

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Comment

The title compound, C₁₁H₁₁ON₂F, is the key intermediate in the synthesis of a new kind of antifungal drug (Porretta *et al.*, 1993). As a part of our ongoing studies (Tao *et al.*, 2007; Liu *et al.*, 2011), the crystal structure determination of the title compound has been carried out in order to elucidate its molecular conformation. The molecular structure of the title compound is shown in Fig. 1. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The dihedral angle between the mean planes of the two rings is 1.30 (4)°. In the crystal structure, intermolecular O—H···N hydrogen bonds (Table 1) link the molecules in chains along the *b* axis.

Experimental

A mixture of 1-(4-fluorophenyl)-2-(1*H*-imidazol-1-yl)ethanone (2.04 g, 10 mol), sodium borohydride (0.756 g, 20 mmol) and 30 ml dry ethanol was refluxed for 3 h. After solvent evaporation, the mixture was neutralized with dilute hydrochloric acid and then refluxed for 30 min. After the mixture was cooled, the solution was alkalized with sodium hydroxide, the precipitate was collected, recrystallized with ethanol, and a yellow deposit was obtain (m.p. 410–412 K). Crystals suitable for a X-ray analysis were obtained by dissolving the crude product (1.0 g) in ethanol (30 ml) and then allowing the solution to evaporate slowly at room temperature for about 7 d.

Refinement

The H atom of the hydroxy group was located in a difference Fourier map and was freely refined with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The other H atoms were positioned geometrically with C—H = 0.93 Å (aromatic), 0.97 Å (methylene), and 0.98 Å (methine) and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The absolute structure parameter is meaningless because the compound is a weak anomalous scatterer ($Z < \text{Si, MoK}\alpha$). The Friedel-pair data were merged and the absolute structure parameter was removed from the CIF.

Figures

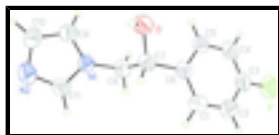


Fig. 1. The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

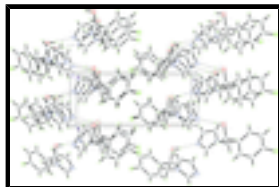


Fig. 2. A packing diagram of the title compound viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

1-(4-Fluorophenyl)-2-(1H-imidazol-1-yl)ethanol

Crystal data

$C_{11}H_{11}FN_2O$	$F(000) = 216$
$M_r = 206.22$	$D_x = 1.368 \text{ Mg m}^{-3}$
Monoclinic, $P2_1$	Melting point: 410 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 7.1220 (14) \text{ \AA}$	Cell parameters from 25 reflections
$b = 5.4690 (11) \text{ \AA}$	$\theta = 9\text{--}14^\circ$
$c = 12.981 (3) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$\beta = 98.13 (3)^\circ$	$T = 293 \text{ K}$
$V = 500.53 (19) \text{ \AA}^3$	Block, colourless
$Z = 2$	$0.30 \times 0.20 \times 0.10 \text{ mm}$

Data collection

Enraf–Nonius CAD-4 diffractometer	876 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube graphite	$R_{\text{int}} = 0.029$
$\omega/2\theta$ scans	$\theta_{\text{max}} = 25.4^\circ$, $\theta_{\text{min}} = 1.6^\circ$
Absorption correction: multi-scan (North <i>et al.</i> , 1968)	$h = 0 \rightarrow 8$
$T_{\text{min}} = 0.970$, $T_{\text{max}} = 0.990$	$k = -6 \rightarrow 6$
1992 measured reflections	$l = -15 \rightarrow 15$
1024 independent reflections	3 standard reflections every 200 reflections
	intensity decay: 1%

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.041$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.124$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.090P)^2]$
1024 reflections	where $P = (F_o^2 + 2F_c^2)/3$
139 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
1 restraint	$\Delta\rho_{\text{max}} = 0.13 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
F	0.9055 (3)	0.3909 (5)	0.52854 (19)	0.0796 (8)
O	0.2786 (4)	-0.0461 (4)	0.19125 (18)	0.0557 (7)
H0A	0.275 (6)	-0.068 (9)	0.125 (3)	0.078*
N1	-0.0381 (3)	0.2845 (5)	0.16087 (19)	0.0445 (6)
C1	0.5787 (5)	0.4661 (7)	0.2920 (3)	0.0524 (8)
H1A	0.5509	0.5790	0.2384	0.063*
C2	0.7277 (5)	0.5097 (7)	0.3702 (3)	0.0575 (9)
H2A	0.8026	0.6486	0.3689	0.069*
N2	-0.2416 (4)	0.3439 (6)	0.0183 (2)	0.0558 (8)
C3	0.7627 (5)	0.3446 (7)	0.4495 (3)	0.0528 (9)
C4	0.6583 (5)	0.1347 (7)	0.4532 (3)	0.0554 (9)
H4A	0.6854	0.0246	0.5080	0.066*
C5	0.5115 (5)	0.0912 (7)	0.3732 (2)	0.0479 (8)
H5A	0.4397	-0.0507	0.3739	0.057*
C6	0.4702 (4)	0.2556 (6)	0.2925 (2)	0.0412 (7)
C7	0.3052 (4)	0.2069 (6)	0.2080 (2)	0.0426 (7)
H7A	0.3311	0.2836	0.1432	0.051*
C8	0.1259 (4)	0.3188 (7)	0.2395 (2)	0.0499 (8)
H8A	0.1010	0.2448	0.3041	0.060*
H8B	0.1460	0.4924	0.2518	0.060*
C9	-0.1609 (5)	0.0911 (7)	0.1518 (3)	0.0538 (9)
H9A	-0.1592	-0.0411	0.1970	0.065*
C10	-0.2855 (5)	0.1288 (8)	0.0645 (3)	0.0538 (9)
H10A	-0.3853	0.0254	0.0395	0.065*
C11	-0.0933 (5)	0.4306 (7)	0.0793 (3)	0.0518 (8)
H11A	-0.0336	0.5770	0.0672	0.062*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F	0.0595 (12)	0.0851 (18)	0.0844 (15)	0.0039 (12)	-0.0237 (11)	-0.0152 (13)
O	0.0673 (15)	0.0462 (14)	0.0498 (13)	0.0048 (12)	-0.0049 (12)	-0.0048 (11)
N1	0.0383 (13)	0.0482 (15)	0.0465 (14)	0.0036 (13)	0.0049 (11)	0.0024 (12)
C1	0.0580 (19)	0.0450 (19)	0.0544 (18)	0.0012 (16)	0.0083 (16)	0.0045 (15)
C2	0.050 (2)	0.0474 (18)	0.074 (2)	-0.0045 (16)	0.0051 (17)	-0.0051 (19)
N2	0.0467 (15)	0.065 (2)	0.0539 (15)	0.0065 (14)	0.0007 (12)	0.0065 (15)
C3	0.0438 (17)	0.054 (2)	0.0572 (19)	0.0073 (16)	-0.0035 (14)	-0.0126 (17)

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C4	0.063 (2)	0.056 (2)	0.0449 (18)	0.0105 (18)	-0.0012 (15)	0.0034 (16)
C5	0.0486 (17)	0.0496 (19)	0.0452 (16)	0.0010 (16)	0.0057 (14)	0.0024 (15)
C6	0.0384 (15)	0.0433 (18)	0.0426 (16)	0.0063 (13)	0.0084 (12)	-0.0042 (13)
C7	0.0459 (16)	0.0440 (17)	0.0374 (15)	0.0043 (13)	0.0041 (13)	0.0003 (13)
C8	0.0492 (18)	0.053 (2)	0.0474 (17)	0.0050 (17)	0.0047 (14)	-0.0054 (16)
C9	0.0556 (19)	0.053 (2)	0.0545 (19)	-0.0056 (16)	0.0128 (16)	0.0074 (16)
C10	0.0409 (16)	0.066 (2)	0.0550 (18)	-0.0048 (16)	0.0077 (15)	-0.0031 (18)
C11	0.0437 (16)	0.0496 (19)	0.062 (2)	0.0009 (16)	0.0054 (15)	0.0104 (16)

Geometric parameters (Å, °)

F—C3	1.362 (4)	C4—C5	1.387 (5)
O—C7	1.409 (5)	C4—H4A	0.9300
O—H0A	0.86 (4)	C5—C6	1.380 (5)
N1—C11	1.340 (4)	C5—H5A	0.9300
N1—C9	1.367 (5)	C6—C7	1.514 (4)
N1—C8	1.450 (4)	C7—C8	1.523 (4)
C1—C2	1.382 (5)	C7—H7A	0.9800
C1—C6	1.387 (5)	C8—H8A	0.9700
C1—H1A	0.9300	C8—H8B	0.9700
C2—C3	1.365 (5)	C9—C10	1.353 (5)
C2—H2A	0.9300	C9—H9A	0.9300
N2—C11	1.316 (4)	C10—H10A	0.9300
N2—C10	1.376 (5)	C11—H11A	0.9300
C3—C4	1.372 (6)		
C7—O—H0A	106 (3)	C1—C6—C7	121.2 (3)
C11—N1—C9	106.3 (3)	O—C7—C6	111.0 (3)
C11—N1—C8	126.6 (3)	O—C7—C8	109.6 (3)
C9—N1—C8	127.0 (3)	C6—C7—C8	109.2 (2)
C2—C1—C6	120.6 (3)	O—C7—H7A	109.0
C2—C1—H1A	119.7	C6—C7—H7A	109.0
C6—C1—H1A	119.7	C8—C7—H7A	109.0
C3—C2—C1	118.6 (4)	N1—C8—C7	112.4 (3)
C3—C2—H2A	120.7	N1—C8—H8A	109.1
C1—C2—H2A	120.7	C7—C8—H8A	109.1
C11—N2—C10	105.0 (3)	N1—C8—H8B	109.1
C2—C3—F	118.8 (3)	C7—C8—H8B	109.1
C2—C3—C4	122.5 (3)	H8A—C8—H8B	107.9
F—C3—C4	118.6 (3)	C10—C9—N1	106.9 (3)
C3—C4—C5	118.2 (3)	C10—C9—H9A	126.6
C3—C4—H4A	120.9	N1—C9—H9A	126.6
C5—C4—H4A	120.9	C9—C10—N2	109.5 (3)
C6—C5—C4	120.9 (3)	C9—C10—H10A	125.3
C6—C5—H5A	119.5	N2—C10—H10A	125.3
C4—C5—H5A	119.5	N2—C11—N1	112.4 (3)
C5—C6—C1	119.1 (3)	N2—C11—H11A	123.8
C5—C6—C7	119.7 (3)	N1—C11—H11A	123.8
C6—C1—C2—C3	-1.7 (5)	C1—C6—C7—C8	-89.0 (3)
C1—C2—C3—F	-177.9 (3)	C11—N1—C8—C7	-87.2 (4)

C1—C2—C3—C4	1.5 (5)	C9—N1—C8—C7	89.0 (4)
C2—C3—C4—C5	-0.3 (5)	O—C7—C8—N1	-59.6 (4)
F—C3—C4—C5	179.0 (3)	C6—C7—C8—N1	178.6 (3)
C3—C4—C5—C6	-0.6 (5)	C11—N1—C9—C10	0.1 (3)
C4—C5—C6—C1	0.3 (5)	C8—N1—C9—C10	-176.7 (3)
C4—C5—C6—C7	-178.1 (3)	N1—C9—C10—N2	0.2 (4)
C2—C1—C6—C5	0.9 (5)	C11—N2—C10—C9	-0.5 (4)
C2—C1—C6—C7	179.3 (3)	C10—N2—C11—N1	0.6 (4)
C5—C6—C7—O	-31.6 (4)	C9—N1—C11—N2	-0.5 (4)
C1—C6—C7—O	150.0 (3)	C8—N1—C11—N2	176.3 (3)
C5—C6—C7—C8	89.4 (3)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O-H0A\cdots N2^i$	0.87 (4)	1.90 (4)	2.762 (4)	171 (5)

Symmetry codes: (i) $-x, y-1/2, -z$.

Fig. 1

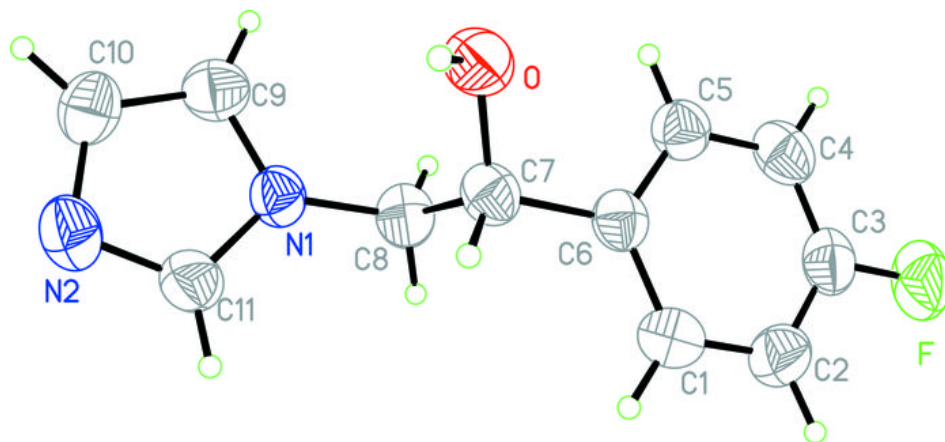


Fig. 2

