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Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.028
 wR factor = 0.070
Data-to-parameter ratio = 8.8

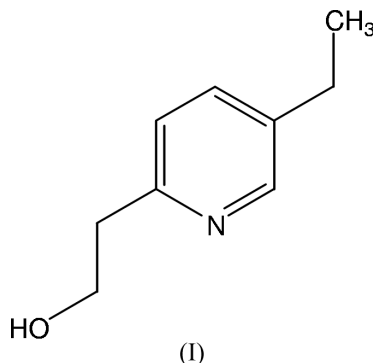
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

2-(5-Ethylpyridin-2-yl)ethanol

The title compound, $\text{C}_9\text{H}_{13}\text{NO}$, is the key intermediate for the synthesis of the antidiabetic drug pioglitazone and it is used as a versatile intermediate in the synthesis of a number of biologically active novel heterocycles. Both side-chains are located on the same side of the aromatic ring. The molecules are connected by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds into ribbons which show a herring-bone-like pattern.

Comment

The title compound, (I), is the key intermediate for the synthesis of the antidiabetic drug pioglitazone and also finds use as a versatile intermediate in the synthesis of a number of biologically active novel heterocycles (Sohda *et al.*, 1982, 1990, 2002).



A perspective view of (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 1.6 plus three updates; MOGUL Version 1.0; Allen, 2002). Both side-chains attached to the pyridyl ring are located on the same side of the aromatic ring. The conformation of the hydroxyethyl chain is *trans* [$\text{C}2-\text{C}21-\text{C}22-\text{O}23 = 176.65(16)^\circ$]. In the crystal structure, the molecules are connected by $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonding between the hydroxy H atom and the N atom of the pyridine ring into ribbons which propagate in the direction of the c axis. These ribbons are arranged in a herring-bone-like pattern (Fig. 2).

Experimental

A mixture of 5-ethyl-2-methylpyridine (12.1 g, 0.1 mol), formaldehyde (4.0 g, 0.13 mol) and a catalytic amount of dibutylamine was heated at 443 K in an autoclave under nitrogen pressure. The product formed was steam-distilled to obtain an oil, which was left overnight in *n*-hexane to produce the title compound. This was recrystallized as hygroscopic colourless prisms from ethanol and the crystals were stored under nitrogen.

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Crystal data

C₉H₁₃NO
M_r = 151.20
 Tetragonal, *P*4₂*c*
a = 14.692 (2) Å
c = 8.0106 (13) Å
V = 1729.1 (4) Å³
Z = 8
D_x = 1.162 Mg m⁻³

Mo *K*α radiation
 Cell parameters from 3889 reflections
 θ = 3.8–25.7°
 μ = 0.08 mm⁻¹
T = 173 (2) K
 Block, colourless
 0.26 × 0.22 × 0.19 mm

Data collection

Stoe IPDS-II two-circle diffractometer
 ω scans
 Absorption correction: none
 4259 measured reflections
 925 independent reflections

777 reflections with *I* > 2σ(*I*)
*R*_{int} = 0.047
 θ_{max} = 25.7°
h = −17 → 15
k = −17 → 13
l = −6 → 9

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.028
wR (*F*²) = 0.070
S = 0.98
 925 reflections
 105 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.11 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.10 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.012 (2)

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O23—H23...N1 ⁱ	0.88 (3)	1.93 (3)	2.802 (2)	171 (3)

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

H atoms were geometrically positioned and refined with fixed individual displacement parameters [*U*_{iso}(H) = 1.2*U*_{eq}(C) or 1.5*U*_{eq}(C_{methyl})] using a riding model [C—H = 0.99, 0.98 and 0.95 Å for methylene, methyl and aromatic CH groups, respectively]. The hydroxy H atom was refined isotropically. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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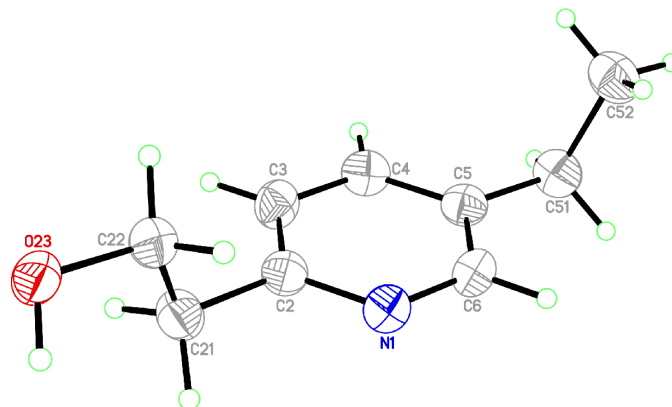


Figure 1

Perspective view of the title compound showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

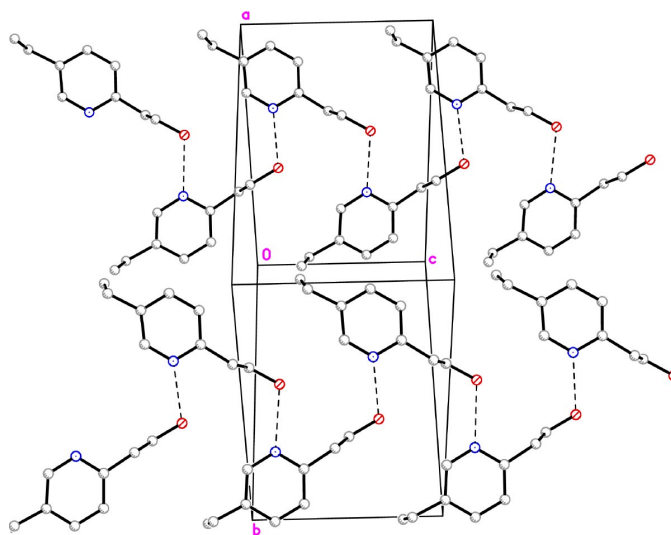


Figure 2

Packing diagram of the title compound, viewed along $(\bar{1}10)$. H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

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