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

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–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.

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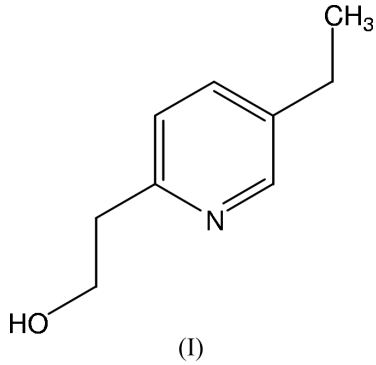
The title compound, $C_9H_{13}NO$, is the key intermediate for the synthesis of the antidiabetic drug pioglitazone and it is used as a versatile intermediate in the synthesis of a number of biologically active novel heterocycles. Both side-chains are located on the same side of the aromatic ring. The molecules are connected by O—H···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).



(I)

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* [C2—C21—C22—O23 = 176.65 (16)°]. In the crystal structure, the molecules are connected by O—H···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.

Crystal data

$C_9H_{13}NO$
$M_r = 151.20$
Tetragonal, $P\bar{4}2_1c$
$a = 14.692\ (2)$ Å
$c = 8.0106\ (13)$ Å
$V = 1729.1\ (4)$ Å^3
$Z = 8$
$D_x = 1.162$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3889 reflections
$\theta = 3.8$–$25.7°$
$\mu = 0.08$ 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 $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 25.7°$
$h = -17 \rightarrow 15$
$k = -17 \rightarrow 13$
$l = -6 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.070$
$S = 0.98$
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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.10$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.012 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
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) = 1.2U_{eq}(C) or 1.5U_{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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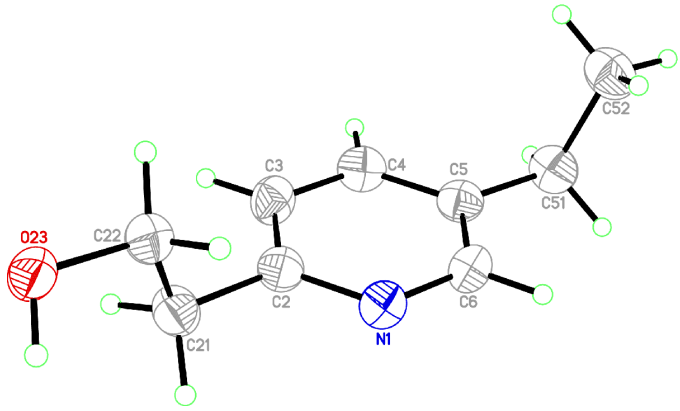

Figure 1
Perspective view of the title compound showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

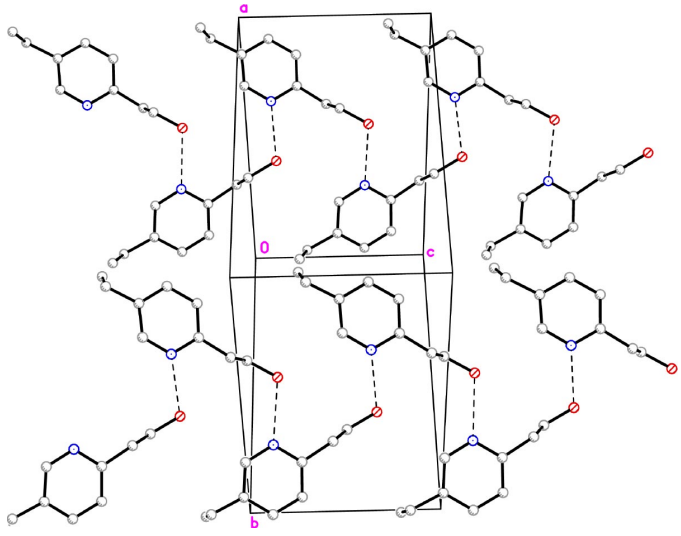

Figure 2
Packing diagram of the title compound, viewed along ($\bar{1}10$). H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

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