

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

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Key indicators

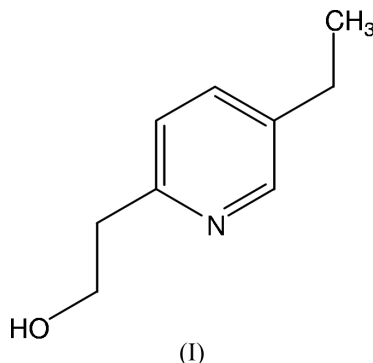
Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.028
 wR factor = 0.070
Data-to-parameter ratio = 8.8

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

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* [$\text{C2}-\text{C21}-\text{C22}-\text{O23} = 176.65(16)^\circ$]. 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.

Received 14 January 2005

Accepted 19 January 2005

Online 29 January 2005

Crystal data

$C_9H_{13}NO$
 $M_r = 151.20$
 Tetragonal, $P4_21c$
 $a = 14.692(2) \text{ \AA}$
 $c = 8.0106(13) \text{ \AA}$
 $V = 1729.1(4) \text{ \AA}^3$
 $Z = 8$
 $D_x = 1.162 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 Cell parameters from 3889 reflections
 $\theta = 3.8\text{--}25.7^\circ$
 $\mu = 0.08 \text{ mm}^{-1}$
 $T = 173(2) \text{ K}$
 Block, colourless
 $0.26 \times 0.22 \times 0.19 \text{ mm}$

Data collection

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

777 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.047$
 $\theta_{\text{max}} = 25.7^\circ$
 $h = -17 \rightarrow 15$
 $k = -17 \rightarrow 13$
 $l = -6 \rightarrow 9$

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

Table 1

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O23-H23\cdots N1^i$	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 [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$] using a riding model [$C-H = 0.99, 0.98$ and 0.95 \AA 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).

References

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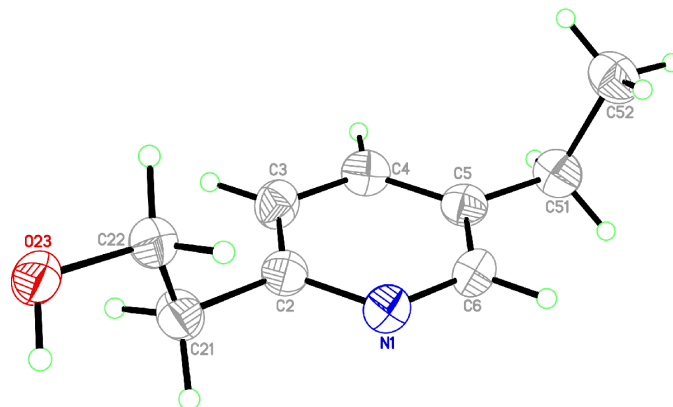


Figure 1

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

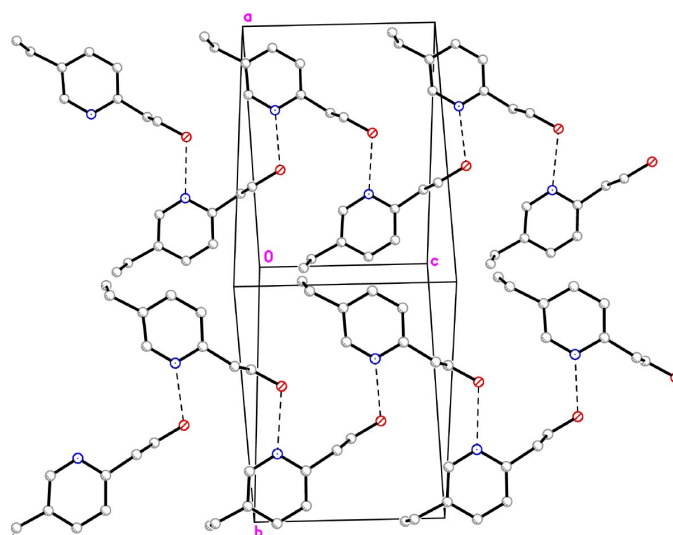


Figure 2

Packing diagram of the title compound, viewed along (110) . H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

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