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2-Ethyl-3-hydroxy-1-morpholinopyridin-4(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.113
Data-to-parameter ratio = 18.4

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

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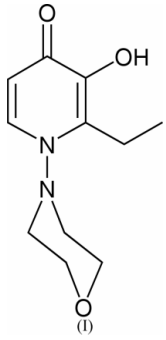
The title compound, $C_{11}H_{16}N_2O_3$, crystallizes in the triclinic space group $P\overline{1}$. The molecules form dimers in the solid state, through hydrogen bonding involving the β-hydroxy ketone functionality.



(I)

Experimental

The title compound was prepared by addition of 4-aminomorpholine (2.92 g, 2.85 mmol) to a stirred solution of 2-ethyl-3-hydroxy-4*H*-pyran-4-one (2.50 g, 1.78 mmol) in H_2O/EtOH (8:4 ml). The reaction was heated at reflux for 72 h, at which point the solvent was removed under vacuum to afford a dark oily solid. Methylene chloride (3 × 5 ml) was used to extract the organic soluble phase and then concentrated to 5 ml and stored at 278 K. The precipitate was collected and washed with thf (2 × 3 ml) to afford a pale brown solid. Yield: 0.44 g (11%); m.p. 531–533 K. The precipitate was recrystallized from cold (278 K) methylene chloride (10 ml).

Crystal data

$C_{11}H_{16}N_2O_3$
M_r = 224.26
Triclinic, $P\overline{1}$
a = 8.4379 (8) Å
b = 8.9209 (9) Å
c = 9.3312 (12) Å
α = 64.020 (3)°
β = 63.198 (2)°
γ = 66.178 (2)°
V = 544.62 (10) Å^3
Z = 2
D_x = 1.368 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 3224 reflections
θ = 2.6–33.1°
μ = 0.10 mm^{-1}
T = 173 (2) K
Irregular, colourless
0.35 × 0.20 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
6121 measured reflections
3838 independent reflections
2543 reflections with $I > 2\sigma(I)$
R_{int} = 0.012
θ_{max} = 32.5°
h = −12 → 12
k = −13 → 12
l = −14 → 14

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.113
S = 0.90
3838 reflections
209 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

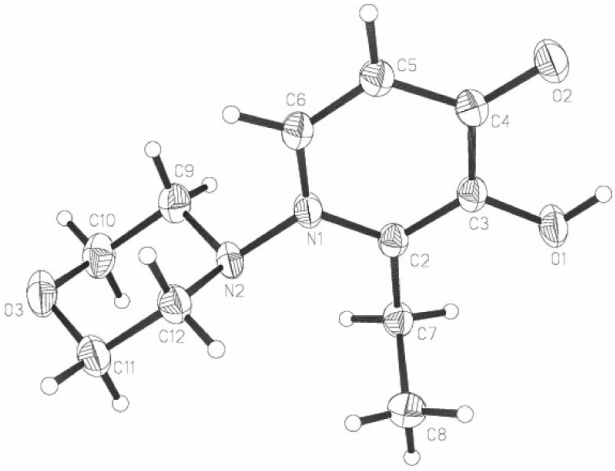


Figure 1
The molecule of the title compound. Ellipsoids are drawn at the 50% probability level. H-atom radii are arbitrary.

All H atoms were refined and C—H distances were in the range 0.879 (16)–1.005 (15) Å.

Data collection: *SMART* (Bruker, 1997–1999); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997–1999) and *SHELXTL* (Sheldrick, 1997*b*); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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References

Bruker (1997–1999). *SMART* and *SAINT*. Versions 5.059. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997*a*). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.