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4-(Quinolin-8-yloxy)butanoic acid

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.073
wR factor = 0.201
Data-to-parameter ratio = 13.8

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

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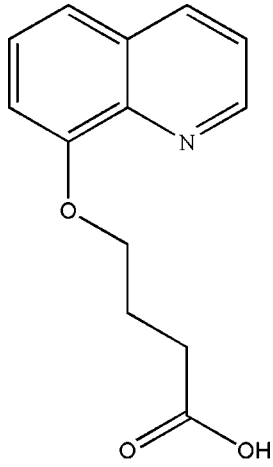
In the title compound, $C_{13}H_{13}NO_3$, the molecules are connected *via* intermolecular O—H···N hydrogen bonds into infinite chains.

Comment

8-Quinolinyloxyacetic acid and its derivatives are known to possess a broad spectrum of biological activities (Kidwai *et al.*, 2000). In the course of our studies on 8-hydroxyquinoline derivatives, the title compound, (I), was synthesized and its crystal structure determined. The bond lengths and angles in (I) fall within their expected ranges (Allen *et al.*, 1987). The conformation along the O1—C1—C2—C3—C4—O3 bond sequence is *trans–trans–*(−)*gauche* (Table 1 and Fig.1). The molecules are connected *via* intermolecular O—H···N hydrogen bonds into one-dimensional helical chains generated by the 2_1 screw axis (Table 2 and Fig. 2).



(I)

Experimental

To a solution of 8-hydroxyquinoline (0.01 mol) in acetonitrile (50 ml), anhydrous potassium carbonate (0.02 mol) and ethyl 4-bromobutanoate were added (0.01 mol). The solution was refluxed for 6 h and then filtered. The filtrate was evaporated under reduced pressure. The residue was dissolved in water and ethanol (1:2 *v*/*v*), then sodium hydroxide (0.02 mol) was added. The solution was refluxed for 24 h, then acidified with dilute HCl. The crude product that precipitated was filtered off and crystals of (I) were recrystallized from a mixture of acetone and ethanol (2:1 *v*/*v*) (m.p. 481 K). Analysis calculated for $C_{13}H_{13}NO_3$: C 67.52, H 5.67, N 6.05%; found: C 67.50, H 5.68, N 6.07%.

Crystal data

$C_{13}H_{13}NO_3$
M_r = 231.24
Monoclinic, $P2_1/n$
a = 10.1256 (5) Å
b = 8.0371 (4) Å
c = 14.9993 (7) Å
β = 107.336 (2)°
V = 1165.20 (10) Å^3
Z = 4
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.46 × 0.32 × 0.20 mm

Data collection

Bruker SMART CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.982
5775 measured reflections
2051 independent reflections
1815 reflections with $I > 2\sigma(I)$
R_{int} = 0.011
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.073
$wR(F^2)$ = 0.201
S = 1.00
2051 reflections
149 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.098P)^2 + 1.2882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected torsion angles (°).

O1—C1—C2—C3	169.5 (3)	C2—C3—C4—O3	−67.7 (3)
C1—C2—C3—C4	−169.5 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	1.93	2.753 (3)	177

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

All H atoms were placed in idealized locations (C—H = 0.93–0.97 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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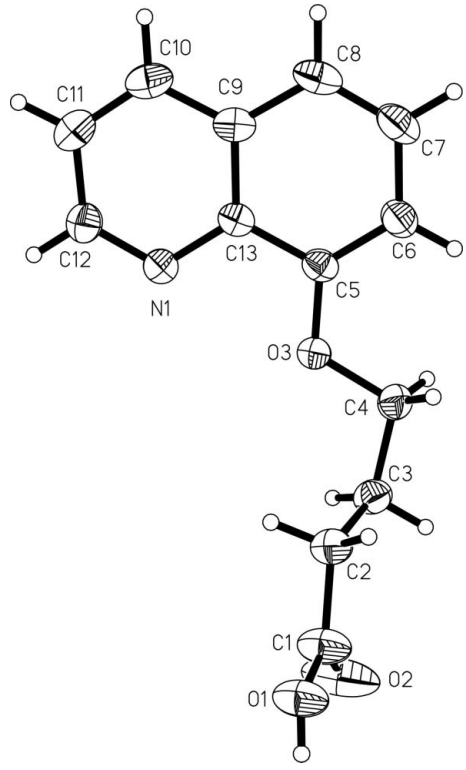

Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level (arbitrary spheres for the H atoms).

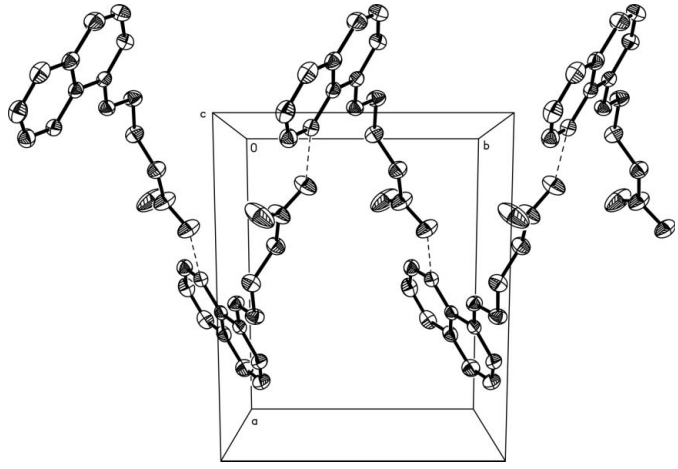

Figure 2
Detail of (I) showing part of a helical hydrogen-bonded chain. H atoms have been omitted for clarity and the dashed lines represent the O···N contacts of the hydrogen bonds.

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