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2-[(8-Hydroxyquinolin-5-yl)methoxy]-ethyl acrylate

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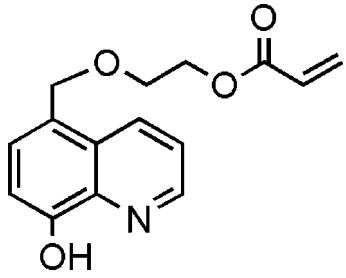
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.220; data-to-parameter ratio = 17.1.

The title compound, $C_{15}H_{15}NO_4$, which is a key intermediate in the synthesis of compounds used in organic light-emitting devices, has been synthesized by the reaction of 5-(chloromethyl)quinolin-8-ol hydrochloride with 2-hydroxyethyl acrylate. Molecules in the solid state are linked by O—H···N intermolecular hydrogen bonds to generate centrosymmetric dimers.

Related literature

The synthesis of 5-(chloromethyl)quinolin-8-ol hydrochloride is described by Burckhalter & Leib (1961). For related literature, see: Tang & VanSlyke (1987); Larson (1970).



Experimental

Crystal data

$C_{15}H_{15}NO_4$
M_r = 273.29
Triclinic, $P\overline{1}$
a = 4.5271 (4) Å
b = 12.1573 (13) Å
c = 12.6900 (11) Å
α = 84.100 (3)°
β = 83.393 (2)°
γ = 87.628 (3)°
V = 689.80 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 296 (1) K
0.50 × 0.50 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.875, T_{max} = 0.990
6815 measured reflections
3113 independent reflections
1338 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.220
S = 1.00
3113 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.83	2.25	2.739 (3)	118
O1—H1···N1^{i}	0.83	2.30	2.894 (3)	129

Symmetry code: (i) $-x, -y+1, -z$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2035).

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supplementary materials

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2-[(8-Hydroxyquinolin-5-yl)methoxy]ethyl acrylate

C.-J. Xu, B.-G. Li, J.-T. Wan and Z.-Y. Bu

Comment

8-Hydroxyquinoline and its derivatives have aroused great interest since the first efficient organic light-emitting diode (OLED), based on aluminium quinolate, was reported by Tang & VanSlyke (1987). Presently, metaloquinolates are considered to be one of the most reliable electro-transporting and emitting materials used in molecular-based OLEDs due to their thermal stability, their high fluorescence yields, and their excellent electron-transporting capability. We report here the preparation and crystal structure of the title compound, (I) (Fig. 1), which is a key intermediate in the synthesis of such compounds used in organic light emitting-devices.

The structure of (I) is composed of two nearly planar moieties: The quinoline ring including oxygen atom O1 and C10, and the ester moiety with the atoms O3, O4 and C11 to C15, which are also nearly coplanar with an r.m.s. deviation from the mean plane of only 0.003 (4) Å. The two planes are connected to each other *via* the ether oxygen atom O2. The dihedral angle between the two planes is 106.6 (2)°.

The hydroxyl group forms two O—H···N hydrogen bonds with the pyridine nitrogen atom, one intramolecular, the other intermolecular to generate centroymmetric dimers as shown in Fig. 2.

Experimental

Into a 100 ml, three-necked, round-bottom flask fitted with a magnetic stirrer, a reflux condenser, and an argon inlet were added 1.78 g (0.0217 mol) of sodium acetate, 0.02 g of hydroquinone, and 20 g of 2-hydroxyethyl acrylate. The reaction solution was stirred at 323 K for 2 h, and then 5.0 g (0.0217 mol) of 5-(chloromethyl)quinolin-8-ol hydrochloride (Burckhalter & Leib, 1961) were added to the solution. The suspension was heated to 363 K for another 10 h. After cooling to room temperature the complex was poured into cool water and dissolved. The solution was neutralized with dilute ammonia. The precipitate was washed with a large amount of water, collected by filtration, and dried to produce 5.1 g (86.1%) of (I) as a grey solid. After four recrystallizations from petroleum ether, a white, flocculent solid was obtained (55.3% yield). A single-crystal suitable for X-ray structure analysis was obtained by slow evaporation of methanolic solution at room temperature (m.p. 331–332 K).

Refinement

The hydroxyl hydrogen atom was located in a difference Fourier map and was refined isotropically. All other H atoms were placed in calculated positions, with C—H = 0.97 (sp^3) or 0.93 Å (sp^2), and were refined using a riding model with U_{iso}(H) = 1.2U_{eq} of the carrier atoms.

Figures

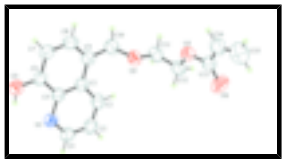

Fig. 1. The molecular structure of (I), with atom labels and 40% probability displacement ellipsoids for non-H atoms.

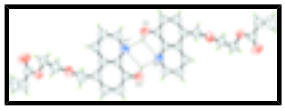

Fig. 2. Hydrogen bonding in (I). Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen bonding have been omitted. Symmetry code: (i) −*x*, 1 − *y*, −*z*.

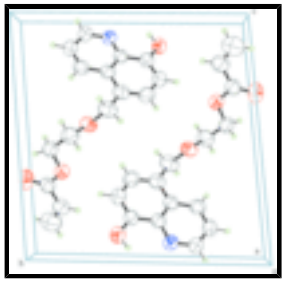

Fig. 3. Packing diagram of a unit cell of (I).

2-[(8-Hydroxyquinolin-5-yl)methoxy]ethyl acrylate

Crystal data

$C_{15}H_{15}NO_4$	$Z = 2$
$M_r = 273.29$	$F_{000} = 288.00$
Triclinic, $P\overline{1}$	$D_x = 1.316$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71075$ Å
$a = 4.5271$ (4) Å	Cell parameters from 3680 reflections
$b = 12.1573$ (13) Å	$\theta = 3.3$–$27.5°$
$c = 12.6900$ (11) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 84.100$ (3)°	$T = 296$ (1) K
$\beta = 83.393$ (2)°	Platelet, colorless
$\gamma = 87.628$ (3)°	0.50 × 0.50 × 0.10 mm
$V = 689.80$ (11) Å^3	

Data collection

Rigaku R-AXIS RAPID diffractometer	1338 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	$R_{int} = 0.031$
ω scans	$\theta_{max} = 27.5°$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$h = -5 \rightarrow 5$
$T_{min} = 0.875$, $T_{max} = 0.990$	$k = -15 \rightarrow 15$
6815 measured reflections	$l = -16 \rightarrow 16$
3113 independent reflections	

Refinement

Refinement on F^2	$w = 1/[0.0030F_o^2 + 1.0000\sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)] = 0.051$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.220$	$\Delta\rho_{max} = 0.34$ e Å^{-3}
$S = 1.00$	$\Delta\rho_{min} = -0.34$ e Å^{-3}
3113 reflections	Extinction correction: Larson (1970)
182 parameters	Extinction coefficient: 168 (39)
H-atom parameters constrained	

Special details

Refinement. Refinement using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (S) are based on F^2. *R*-factor (gt) are based on F. The threshold expression of $F^2 > 2.0$ sigma(F^2) is used only for calculating *R*-factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.0891 (4)	0.61703 (16)	0.10402 (14)	0.0755 (6)
O2	0.6541 (4)	0.29041 (17)	0.45276 (13)	0.0667 (5)
O3	0.4968 (4)	0.15686 (16)	0.64974 (14)	0.0701 (6)
O4	0.2977 (6)	−0.0087 (2)	0.6857 (2)	0.1069 (9)
N1	0.2448 (5)	0.40141 (19)	0.07426 (16)	0.0623 (7)
C1	0.5221 (5)	0.3869 (2)	0.2303 (2)	0.0587 (8)
C2	0.5964 (6)	0.2754 (2)	0.2145 (2)	0.0668 (9)
C3	0.4928 (7)	0.2319 (2)	0.1307 (2)	0.0754 (10)
C4	0.3236 (7)	0.2973 (2)	0.0635 (2)	0.0711 (9)
C5	0.3467 (5)	0.4457 (2)	0.1581 (2)	0.0556 (7)
C6	0.2578 (6)	0.5583 (2)	0.1708 (2)	0.0622 (8)
C7	0.3515 (7)	0.6063 (2)	0.2540 (2)	0.0715 (9)
C8	0.5241 (7)	0.5477 (2)	0.3246 (2)	0.0733 (10)
C9	0.6153 (5)	0.4395 (2)	0.3164 (2)	0.0629 (8)
C10	0.8091 (6)	0.3802 (2)	0.3917 (2)	0.0781 (10)
C11	0.8451 (7)	0.2132 (2)	0.5016 (2)	0.0773 (10)
C12	0.6695 (7)	0.1196 (2)	0.5567 (2)	0.0748 (9)
C13	0.3217 (7)	0.0839 (2)	0.7083 (2)	0.0726 (9)
C14	0.1599 (8)	0.1311 (3)	0.8001 (2)	0.0835 (11)
C15	−0.0322 (9)	0.0750 (4)	0.8663 (3)	0.1161 (16)
H1	0.0782	0.5787	0.0546	0.092*
H2	0.7126	0.2325	0.2599	0.080*
H3	0.5366	0.1585	0.1191	0.091*
H4	0.2607	0.2656	0.0066	0.085*
H7	0.2976	0.6797	0.2629	0.086*
H8	0.5813	0.5831	0.3803	0.088*
H14	0.1953	0.2035	0.8116	0.100*
H101	0.9864	0.3516	0.3519	0.094*

H102	0.8654	0.4312	0.4394	0.094*
H111	0.9436	0.2478	0.5530	0.093*
H112	0.9930	0.1862	0.4480	0.093*
H121	0.5378	0.0951	0.5092	0.090*
H122	0.8026	0.0588	0.5779	0.090*
H151	−0.0699	0.0025	0.8558	0.139*
H152	−0.1319	0.1073	0.9241	0.139*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0986 (16)	0.0577 (13)	0.0719 (12)	0.0074 (11)	−0.0178 (11)	−0.0098 (10)
O2	0.0603 (11)	0.0763 (13)	0.0623 (10)	−0.0031 (10)	−0.0095 (8)	0.0019 (9)
O3	0.0928 (14)	0.0586 (12)	0.0611 (10)	−0.0028 (11)	−0.0145 (10)	−0.0095 (9)
O4	0.145 (2)	0.0593 (15)	0.1153 (19)	−0.0103 (15)	−0.0043 (16)	−0.0140 (13)
N1	0.0747 (15)	0.0571 (15)	0.0546 (12)	−0.0037 (12)	−0.0009 (11)	−0.0095 (10)
C1	0.0571 (15)	0.0613 (18)	0.0553 (14)	−0.0103 (13)	0.0039 (12)	−0.0030 (12)
C2	0.0669 (17)	0.070 (2)	0.0606 (16)	0.0044 (15)	−0.0003 (13)	−0.0017 (14)
C3	0.096 (2)	0.0566 (19)	0.0709 (18)	0.0075 (16)	0.0014 (17)	−0.0076 (15)
C4	0.091 (2)	0.0592 (19)	0.0640 (16)	0.0028 (16)	−0.0084 (15)	−0.0127 (14)
C5	0.0545 (15)	0.0578 (17)	0.0531 (13)	−0.0072 (12)	0.0007 (12)	−0.0033 (12)
C6	0.0695 (18)	0.0549 (18)	0.0604 (15)	−0.0061 (14)	0.0000 (13)	−0.0036 (13)
C7	0.085 (2)	0.0590 (19)	0.0722 (17)	−0.0080 (16)	−0.0098 (16)	−0.0104 (15)
C8	0.079 (2)	0.077 (2)	0.0666 (18)	−0.0217 (17)	−0.0076 (15)	−0.0132 (15)
C9	0.0529 (15)	0.075 (2)	0.0591 (15)	−0.0137 (14)	−0.0018 (12)	−0.0004 (14)
C10	0.0662 (18)	0.097 (2)	0.0704 (18)	−0.0230 (17)	−0.0071 (14)	0.0041 (17)
C11	0.073 (2)	0.086 (2)	0.0723 (18)	0.0129 (18)	−0.0169 (15)	−0.0052 (16)
C12	0.094 (2)	0.068 (2)	0.0656 (16)	0.0164 (17)	−0.0193 (15)	−0.0139 (14)
C13	0.088 (2)	0.062 (2)	0.0701 (17)	0.0063 (16)	−0.0251 (15)	−0.0031 (15)
C14	0.096 (2)	0.083 (2)	0.0724 (19)	0.0083 (19)	−0.0202 (18)	−0.0018 (17)
C15	0.110 (3)	0.134 (3)	0.099 (2)	0.003 (2)	−0.006 (2)	0.003 (2)

Geometric parameters (Å, °)

O1—C6	1.338 (3)	C11—C12	1.483 (4)
O2—C10	1.432 (3)	C13—C14	1.459 (4)
O2—C11	1.396 (3)	C14—C15	1.301 (5)
O3—C12	1.442 (3)	O1—H1	0.826
O3—C13	1.325 (3)	C2—H2	0.930
O4—C13	1.202 (4)	C3—H3	0.930
N1—C4	1.317 (3)	C4—H4	0.930
N1—C5	1.373 (3)	C7—H7	0.930
C1—C2	1.412 (4)	C8—H8	0.930
C1—C5	1.403 (3)	C10—H101	0.970
C1—C9	1.432 (4)	C10—H102	0.970
C2—C3	1.372 (4)	C11—H111	0.970
C3—C4	1.381 (4)	C11—H112	0.970
C5—C6	1.431 (4)	C12—H121	0.970
C6—C7	1.373 (4)	C12—H122	0.970

C7—C8	1.380 (4)	C14—H14	0.930
C8—C9	1.374 (4)	C15—H151	0.930
C9—C10	1.483 (4)	C15—H152	0.930
C10—O2—C11	112.6 (2)	C3—C2—H2	120.8
C12—O3—C13	116.8 (2)	C2—C3—H3	120.0
C4—N1—C5	115.8 (2)	C4—C3—H3	120.0
C2—C1—C5	117.1 (2)	N1—C4—H4	117.7
C2—C1—C9	122.6 (2)	C3—C4—H4	117.7
C5—C1—C9	120.3 (2)	C6—C7—H7	119.4
C1—C2—C3	118.3 (2)	C8—C7—H7	119.4
C2—C3—C4	120.0 (2)	C7—C8—H8	118.5
N1—C4—C3	124.7 (2)	C9—C8—H8	118.5
N1—C5—C1	124.1 (2)	O2—C10—H101	109.3
N1—C5—C6	115.9 (2)	O2—C10—H102	109.3
C1—C5—C6	120.0 (2)	C9—C10—H101	109.3
O1—C6—C5	121.9 (2)	C9—C10—H102	109.3
O1—C6—C7	119.8 (2)	H101—C10—H102	109.5
C5—C6—C7	118.3 (2)	O2—C11—H111	109.6
C6—C7—C8	121.2 (2)	O2—C11—H112	109.6
C7—C8—C9	123.0 (3)	C12—C11—H111	109.6
C1—C9—C8	117.2 (2)	C12—C11—H112	109.6
C1—C9—C10	121.3 (2)	H111—C11—H112	109.5
C8—C9—C10	121.5 (2)	O3—C12—H121	109.7
O2—C10—C9	110.1 (2)	O3—C12—H122	109.7
O2—C11—C12	109.1 (2)	C11—C12—H121	109.7
O3—C12—C11	108.4 (2)	C11—C12—H122	109.7
O3—C13—O4	123.1 (2)	H121—C12—H122	109.5
O3—C13—C14	111.7 (2)	C13—C14—H14	119.0
O4—C13—C14	125.2 (3)	C15—C14—H14	119.0
C13—C14—C15	121.9 (3)	C14—C15—H151	120.0
C6—O1—H1	106.0	C14—C15—H152	120.0
C1—C2—H2	120.8	H151—C15—H152	120.0
C10—O2—C11—C12	−176.1 (2)	C9—C1—C5—C6	−0.6 (3)
C11—O2—C10—C9	162.6 (2)	C1—C2—C3—C4	0.8 (4)
C12—O3—C13—O4	−1.7 (4)	C2—C3—C4—N1	−1.3 (4)
C12—O3—C13—C14	179.8 (2)	N1—C5—C6—O1	−0.9 (3)
C13—O3—C12—C11	179.1 (2)	N1—C5—C6—C7	179.5 (2)
C4—N1—C5—C1	−0.5 (3)	C1—C5—C6—O1	−179.6 (2)
C4—N1—C5—C6	−179.1 (2)	C1—C5—C6—C7	0.7 (3)
C5—N1—C4—C3	1.1 (4)	O1—C6—C7—C8	179.6 (2)
C2—C1—C5—N1	0.0 (3)	C5—C6—C7—C8	−0.7 (4)
C2—C1—C5—C6	178.6 (2)	C6—C7—C8—C9	0.6 (4)
C5—C1—C2—C3	−0.2 (3)	C7—C8—C9—C1	−0.4 (4)
C2—C1—C9—C8	−178.7 (2)	C7—C8—C9—C10	177.9 (2)
C2—C1—C9—C10	2.9 (3)	C1—C9—C10—O2	−65.9 (3)
C9—C1—C2—C3	179.0 (2)	C8—C9—C10—O2	115.8 (3)
C5—C1—C9—C8	0.4 (3)	O2—C11—C12—O3	−72.1 (3)
C5—C1—C9—C10	−178.0 (2)	O3—C13—C14—C15	177.6 (3)

C9—C1—C5—N1	−179.2 (2)	O4—C13—C14—C15	−0.8 (6)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1	0.83	2.25	2.739 (3)	118
O1—H1···N1^{i}	0.83	2.30	2.894 (3)	129

Symmetry codes: (i) −*x*, −*y*+1, −*z*.

Fig. 1

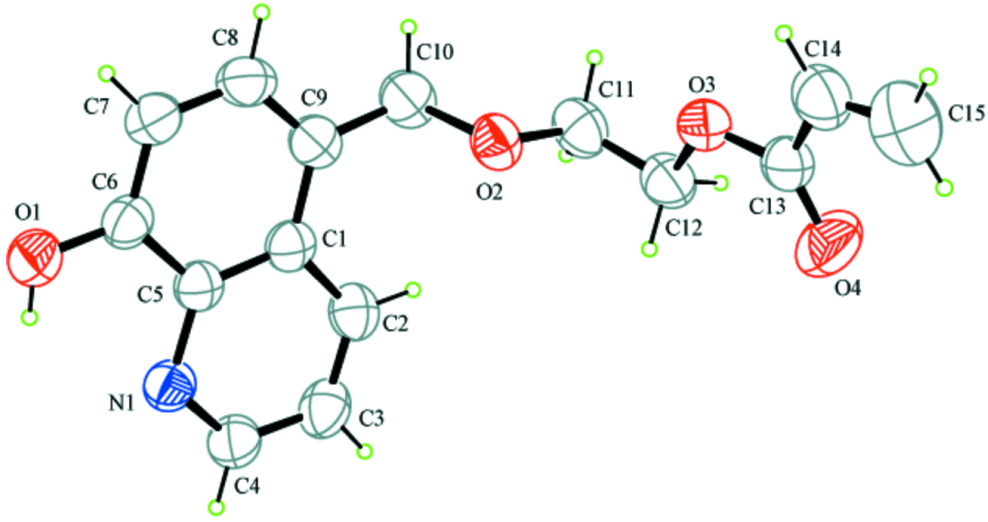

Fig. 2

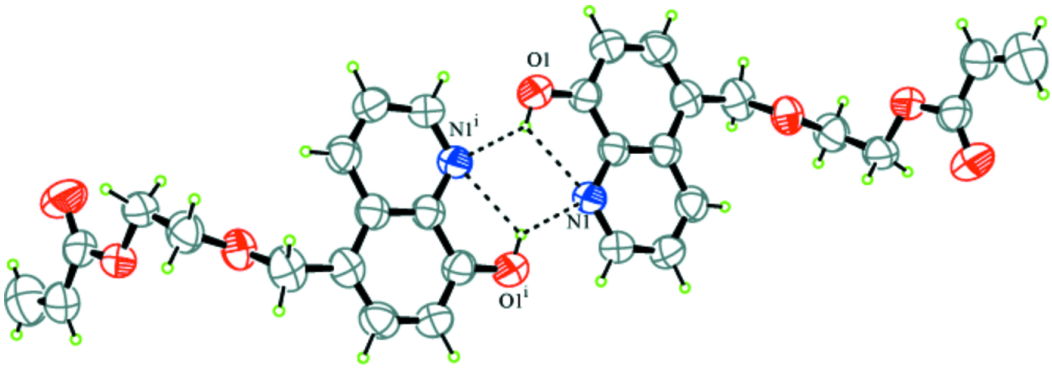

Fig. 3