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2-Chloro-3-hydroxymethyl-6-methoxyquinoline

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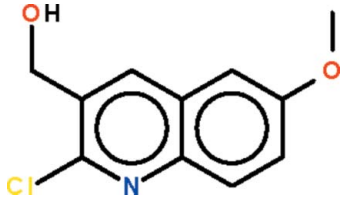
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 17.0.

All the non-H atoms of the title compound, $C_{11}H_{10}ClNO_2$, are roughly coplanar (r.m.s. deviation = 0.058 Å). In the crystal, adjacent molecules are linked by an O—H···N hydrogen bond, generating chains running along the *a* axis.

Related literature

Substituted quinoline-3-carbaldehydes are intermediates for annelation and functional group modification; for a review of the synthesis of quinolines by the Vilsmeier–Haack reaction, see: Meth-Cohn (1993).



Experimental

Crystal data

$C_{11}H_{10}ClNO_2$
M_r = 223.65
Monoclinic, $P2_1/n$
a = 6.9738 (3) Å
b = 21.4668 (9) Å
c = 7.3479 (4) Å
β = 108.220 (5)°
V = 1044.87 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 293 K
0.28 × 0.21 × 0.20 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.910, T_{max} = 0.935
11517 measured reflections
2348 independent reflections
1487 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 0.97
2348 reflections
138 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1^{i}	0.82	2.16	2.913 (2)	153

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5140).

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supplementary materials

Acta Cryst. (2010). E**66**, o201 [**doi:10.1107/S1600536809054051**]

2-Chloro-3-hydroxymethyl-6-methoxyquinoline

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Experimental

2-Chloro-8-methoxyquinoline-3-carbaldehyde (220 mg, 1 mmol), sodium borohydride (38 mg, 1 mmol) and a catalytic amount of montmorillonite K-10 were placed in a beaker. The contents were irradiated at 500 W for 5 min. The product was dissolved in ethyl acetate and the residue removed by filtration. The filtrate was subjected to column chromatography on silica, and ethyl acetate/petroleum ether was used as the eluant. The solvent was evaporated and the residue recrystallized from chloroform to give colorless crystals.

Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93–0.97, O–H 0.82 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C,*O*).

Figures

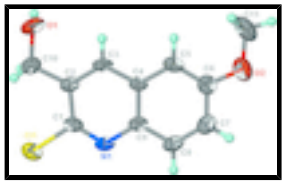

Fig. 1. Anisotropic displacement ellipsoid plot (Barbour, 2001) of $C_{11}H_{10}ClNO_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

2-Chloro-3-hydroxymethyl-6-methoxyquinoline

Crystal data

$C_{11}H_{10}ClNO_2$	$F(000) = 464$
$M_r = 223.65$	$D_x = 1.422$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 1941 reflections
$a = 6.9738$ (3) Å	$\theta = 3.1$–$25.5°$
$b = 21.4668$ (9) Å	$\mu = 0.34$ mm^{-1}
$c = 7.3479$ (4) Å	$T = 293$ K
$\beta = 108.220$ (5)°	Block, colorless
$V = 1044.87$ (8) Å^3	0.28 × 0.21 × 0.20 mm
$Z = 4$	

Data collection

Bruker SMART area-detector	2348 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

graphite

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

T_{min} = 0.910, T_{max} = 0.935

11517 measured reflections

1487 reflections with $I > 2\sigma(I)$

R_{int} = 0.035

θ_{max} = 27.5°, θ_{min} = 3.1°

$h = -9 \rightarrow 8$

$k = -26 \rightarrow 27$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.041

$wR(F^2)$ = 0.108

S = 0.97

2348 reflections

138 parameters

0 restraints

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.058P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 0.21 e Å^{-3}

$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.33210 (8)	0.65210 (2)	0.10064 (7)	0.0648 (2)
O1	0.97027 (18)	0.59162 (7)	0.33602 (19)	0.0672 (4)
H1	1.0200	0.5790	0.2554	0.101*
O2	0.4314 (2)	0.29302 (7)	0.3876 (2)	0.0766 (5)
N1	0.2607 (2)	0.53770 (7)	0.16969 (18)	0.0446 (4)
C1	0.4061 (3)	0.57605 (8)	0.1763 (2)	0.0430 (4)
C2	0.6156 (2)	0.56246 (8)	0.2401 (2)	0.0408 (4)
C3	0.6650 (2)	0.50291 (8)	0.2994 (2)	0.0437 (4)
H3	0.8004	0.4916	0.3461	0.052*
C4	0.5149 (2)	0.45775 (8)	0.2917 (2)	0.0390 (4)
C5	0.5600 (3)	0.39542 (9)	0.3483 (2)	0.0494 (5)
H5	0.6935	0.3821	0.3926	0.059*
C6	0.4070 (3)	0.35449 (9)	0.3379 (2)	0.0526 (5)
C7	0.2053 (3)	0.37443 (9)	0.2741 (2)	0.0546 (5)
H7	0.1027	0.3463	0.2698	0.065*
C8	0.1583 (3)	0.43397 (9)	0.2189 (2)	0.0507 (5)
H8	0.0238	0.4463	0.1758	0.061*
C9	0.3120 (2)	0.47761 (8)	0.2261 (2)	0.0405 (4)
C10	0.7702 (3)	0.61178 (9)	0.2442 (3)	0.0528 (5)
H10A	0.7575	0.6240	0.1138	0.063*
H10B	0.7430	0.6482	0.3103	0.063*
C11	0.6296 (4)	0.26820 (11)	0.4324 (4)	0.0912 (8)

H11A	0.6799	0.2747	0.3263	0.137*
H11B	0.6264	0.2244	0.4573	0.137*
H11C	0.7163	0.2887	0.5439	0.137*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0574 (3)	0.0603 (3)	0.0736 (4)	0.0151 (2)	0.0158 (3)	0.0111 (3)
O1	0.0365 (8)	0.0931 (11)	0.0762 (9)	−0.0030 (7)	0.0235 (7)	−0.0079 (8)
O2	0.0887 (12)	0.0522 (9)	0.0807 (10)	0.0010 (8)	0.0147 (8)	0.0016 (7)
N1	0.0306 (8)	0.0591 (9)	0.0412 (8)	0.0057 (7)	0.0069 (6)	−0.0035 (7)
C1	0.0389 (10)	0.0539 (10)	0.0365 (9)	0.0122 (8)	0.0123 (8)	−0.0006 (8)
C2	0.0347 (9)	0.0573 (11)	0.0341 (8)	0.0033 (8)	0.0161 (7)	−0.0036 (8)
C3	0.0277 (9)	0.0628 (11)	0.0403 (9)	0.0106 (8)	0.0103 (7)	−0.0021 (8)
C4	0.0328 (9)	0.0524 (10)	0.0307 (8)	0.0059 (8)	0.0083 (7)	−0.0051 (7)
C5	0.0420 (11)	0.0593 (12)	0.0428 (10)	0.0127 (9)	0.0076 (8)	−0.0032 (9)
C6	0.0589 (13)	0.0534 (12)	0.0427 (10)	−0.0005 (9)	0.0119 (9)	−0.0073 (9)
C7	0.0504 (12)	0.0631 (13)	0.0476 (10)	−0.0115 (10)	0.0115 (9)	−0.0095 (9)
C8	0.0334 (10)	0.0698 (13)	0.0443 (10)	−0.0022 (9)	0.0056 (8)	−0.0093 (9)
C9	0.0334 (9)	0.0559 (11)	0.0304 (8)	0.0047 (8)	0.0070 (7)	−0.0069 (8)
C10	0.0433 (11)	0.0653 (12)	0.0547 (11)	0.0001 (9)	0.0223 (9)	0.0013 (10)
C11	0.113 (2)	0.0600 (14)	0.1016 (18)	0.0275 (14)	0.0342 (16)	0.0121 (13)

Geometric parameters (Å, °)

Cl1—C1	1.7496 (18)	C4—C9	1.411 (2)
O1—C10	1.414 (2)	C5—C6	1.366 (2)
O1—H1	0.8200	C5—H5	0.9300
O2—C6	1.366 (2)	C6—C7	1.403 (3)
O2—C11	1.421 (3)	C7—C8	1.350 (3)
N1—C1	1.295 (2)	C7—H7	0.9300
N1—C9	1.368 (2)	C8—C9	1.412 (2)
C1—C2	1.418 (2)	C8—H8	0.9300
C2—C3	1.360 (2)	C10—H10A	0.9700
C2—C10	1.505 (2)	C10—H10B	0.9700
C3—C4	1.415 (2)	C11—H11A	0.9600
C3—H3	0.9300	C11—H11B	0.9600
C4—C5	1.407 (2)	C11—H11C	0.9600
C10—O1—H1	109.5	C8—C7—C6	120.86 (18)
C6—O2—C11	117.08 (18)	C8—C7—H7	119.6
C1—N1—C9	117.42 (14)	C6—C7—H7	119.6
N1—C1—C2	126.53 (16)	C7—C8—C9	120.44 (17)
N1—C1—Cl1	115.57 (13)	C7—C8—H8	119.8
C2—C1—Cl1	117.90 (14)	C9—C8—H8	119.8
C3—C2—C1	115.52 (16)	N1—C9—C4	121.87 (16)
C3—C2—C10	123.17 (16)	N1—C9—C8	119.38 (15)
C1—C2—C10	121.30 (16)	C4—C9—C8	118.75 (16)
C2—C3—C4	121.42 (16)	O1—C10—C2	112.82 (16)

C2—C3—H3	119.3	O1—C10—H10A	109.0
C4—C3—H3	119.3	C2—C10—H10A	109.0
C5—C4—C9	119.71 (16)	O1—C10—H10B	109.0
C5—C4—C3	123.07 (16)	C2—C10—H10B	109.0
C9—C4—C3	117.21 (15)	H10A—C10—H10B	107.8
C6—C5—C4	119.79 (17)	O2—C11—H11A	109.5
C6—C5—H5	120.1	O2—C11—H11B	109.5
C4—C5—H5	120.1	H11A—C11—H11B	109.5
O2—C6—C5	125.23 (18)	O2—C11—H11C	109.5
O2—C6—C7	114.34 (18)	H11A—C11—H11C	109.5
C5—C6—C7	120.43 (18)	H11B—C11—H11C	109.5
C9—N1—C1—C2	−1.4 (2)	C4—C5—C6—C7	−1.1 (3)
C9—N1—C1—Cl1	179.45 (10)	O2—C6—C7—C8	−179.55 (16)
N1—C1—C2—C3	0.1 (2)	C5—C6—C7—C8	1.1 (3)
Cl1—C1—C2—C3	179.24 (12)	C6—C7—C8—C9	−0.6 (3)
N1—C1—C2—C10	−178.78 (16)	C1—N1—C9—C4	0.9 (2)
Cl1—C1—C2—C10	0.4 (2)	C1—N1—C9—C8	−179.17 (15)
C1—C2—C3—C4	1.7 (2)	C5—C4—C9—N1	179.93 (14)
C10—C2—C3—C4	−179.43 (15)	C3—C4—C9—N1	0.8 (2)
C2—C3—C4—C5	178.76 (15)	C5—C4—C9—C8	0.0 (2)
C2—C3—C4—C9	−2.1 (2)	C3—C4—C9—C8	−179.16 (14)
C9—C4—C5—C6	0.5 (2)	C7—C8—C9—N1	−179.89 (15)
C3—C4—C5—C6	179.60 (16)	C7—C8—C9—C4	0.1 (2)
C11—O2—C6—C5	−7.7 (3)	C3—C2—C10—O1	−6.8 (2)
C11—O2—C6—C7	173.00 (17)	C1—C2—C10—O1	171.94 (14)
C4—C5—C6—O2	179.68 (15)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N1^{i}	0.82	2.16	2.913 (2)	153

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

Fig. 1