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(2-Chloro-8-methylquinolin-3-yl)-methanol

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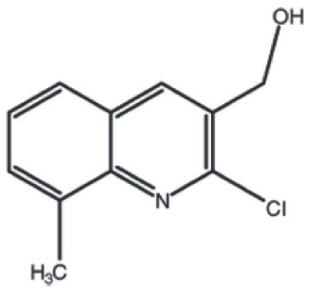
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.006 Å; R factor = 0.061; wR factor = 0.135; data-to-parameter ratio = 13.4.

The molecule of title compound, $C_{11}H_{10}ClNO$, is close to being planar (r.m.s deviation for the non-H atoms = 0.017 Å). In the crystal, molecules interact by way of O—H$\cdots$O hydrogen bonds, generating C(2) chains propagating in [010]. The crystal structure is consolidated by C—H$\cdots\pi$ interactions and aromatic π–π stacking interactions [centroid–centroid distance = 3.661 (2) Å].

Related literature

For a related structure and background references, see: Roopan *et al.* (2010). For a similar structure, see: Khan *et al.* (2009).



Experimental

Crystal data

$C_{11}H_{10}ClNO$
M_r = 207.65
Monoclinic, $P2_1/c$
a = 14.963 (2) Å
b = 4.632 (1) Å
c = 14.469 (2) Å
β = 103.612 (1)°
V = 974.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 290 K
0.40 × 0.24 × 0.11 mm

Data collection

Oxford Xcalibur Eos(Nova) CCD detector diffractometer
Absorption correction: multi-scan (*CrysAlis PRO* RED; Oxford Diffraction, 2009)
T_{min} = 0.871, T_{max} = 0.962
7607 measured reflections
1723 independent reflections
790 reflections with $I > 2\sigma(I)$
R_{int} = 0.167

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.135
S = 0.85
1723 reflections
129 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

Cg1 is a centroid of the N1/C1–C3/C8/C9 ring.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1—H1$O\cdots$O1^{i}	0.82	1.90	2.712 (4)	174
C10—H10$A\cdots Cg1^{ii}$	0.97	2.75	3.557 (4)	141

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

Data collection: *CrysAlis PRO CCD* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO CCD*; data reduction: *CrysAlis PRO RED* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5470).

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supporting information

Acta Cryst. (2010). E**66**, o1543 [doi:10.1107/S1600536810020490]

(2-Chloro-8-methylquinolin-3-yl)methanol

S. Mohana Roopan, F. Nawaz Khan, Rajesh Kumar, Venkatesha R. Hathwar and Mehmet Akkurt

S1. Comment

As part of our program which aimed to develop new selective and environmentally friendly methodologies for the preparation of 2-chloroquinolines (Roopan *et al.*, 2010), we report here crystal structure of the title compound, (I).

The title molecule (I), (Fig. 1), except the hydroxyl and methyl H atoms, close to planar (r.m.s deviation 0.017 Å). The values of the geometric parameters in (I) are comparable to those of some similar structures (Khan *et al.*, 2009).

In the solid-state, the molecules are linked *via* intermolecular O—H···O hydrogen bonds (Table 1, Fig. 2). The crystal structure is further stabilized by an intermolecular C–H···π interactions between the methylene H atom of ethenol substituent and the pyridine ring of an adjacent molecule, with a C10–H10A···$Cg1^{ii}$ separation of 2.75 Å (Table 1, *Cg*1 is the centroid of N1/C1–C3/C8/C9 pyridine ring; symmetry code: (ii) x, $y + 1$, z). In addition, the packing mode results in stabilizing π-π stacking interactions [$Cg1\cdots Cg2^{ii}$ = 3.661 (2) Å, where *Cg*1 and *Cg*2 are the centroids of the N1/C1–C3/C8/C9 and C4–C9 rings].

S2. Experimental

2-Chloro-8-methylquinoline-3-carbaldehyde (206 mg, 1 mmol), sodium borohydride (38 mg, 1 mmol) and catalytic amount of montmorillonite K-10 were taken in an open vessel and the resulting mixture was irradiating at 500 W for 4 min. Ethylacetate was poured into the reaction mixture and filtered off. The filtrated after removal of solvent ethy lacetate was subjected to column chromatography packed with silica and ethyl acetate/petroleum ether was used as the eluant. Colourless plates of (I) were grown by solvent evaporation from a solution of the compound in chloroform.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93- 0.97 Å, and refined a riding model with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C). The value of R_{int} [0.167] is greater than 0.12, which may reflect the poor crystal quality.

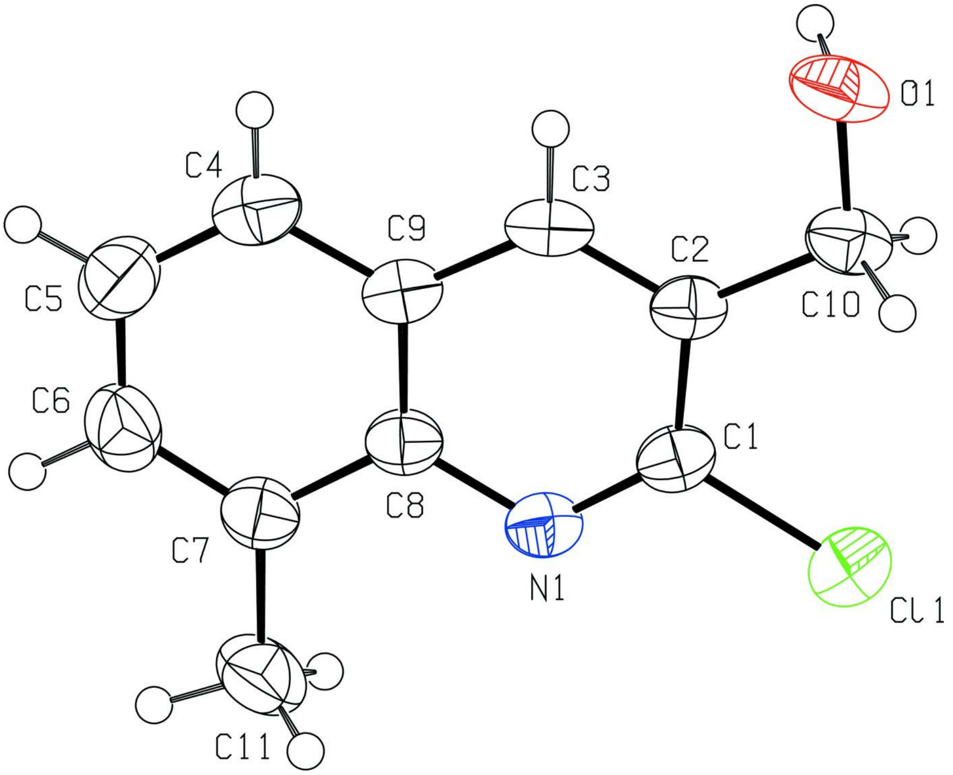

Figure 1

The molecule of (I), showing 50% probability displacement ellipsoids.

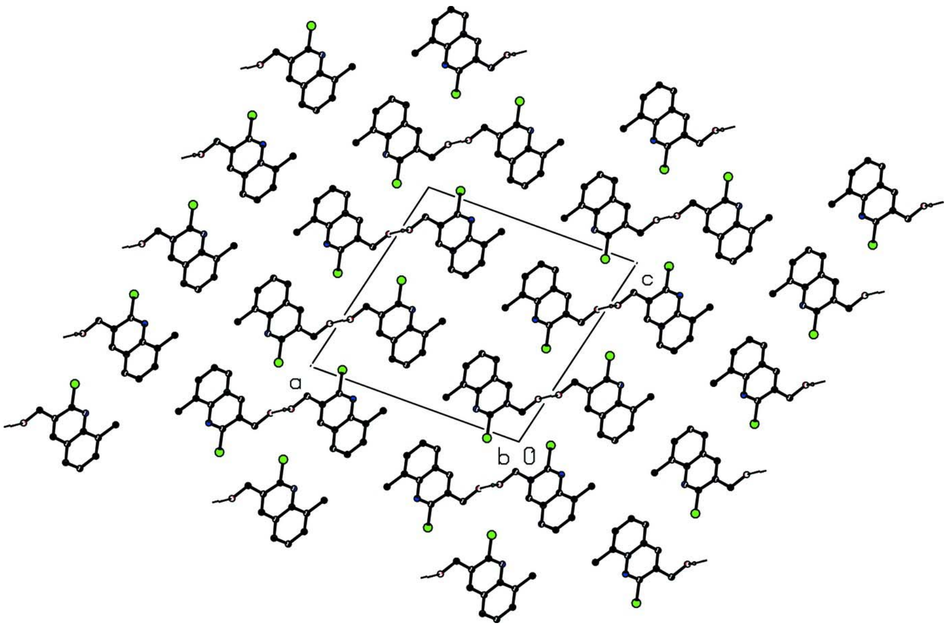

Figure 2

A view of the packing of (I) with intermolecular O–H···O hydrogen bonding down the *b* axis. The H atoms not involved in hydrogen bonds have been omitted for clarity.

(2-Chloro-8-methylquinolin-3-yl)methanol

Crystal data

$C_{11}H_{10}ClNO$
$M_r = 207.65$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.963$ (2) Å
$b = 4.632$ (1) Å
$c = 14.469$ (2) Å
$\beta = 103.612$ (1)°
$V = 974.7$ (3) Å^3
$Z = 4$
$F(000) = 432$
$D_x = 1.415$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 972 reflections
$\theta = 2.0$–20.5°
$\mu = 0.35$ mm^{-1}
$T = 290$ K
Plate, colourless
0.40 × 0.24 × 0.11 mm

Data collection

Oxford Xcalibur Eos(Nova) CCD detector diffractometer
Radiation source: Enhance (Mo) X-ray Source
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrysAlis PRO* RED; Oxford Diffraction, 2009)
$T_{min} = 0.871$, $T_{max} = 0.962$
7607 measured reflections
1723 independent reflections
790 reflections with $I > 2\sigma(I)$
$R_{int} = 0.167$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.9°$
$h = -17 \rightarrow 17$
$k = -5 \rightarrow 5$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.135$
$S = 0.85$
1723 reflections
129 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
$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.13301 (8)	0.6900 (2)	−0.03546 (7)	0.0599 (5)
O1	0.0342 (2)	0.8800 (5)	0.2237 (2)	0.0534 (11)
N1	0.2487 (2)	0.3588 (7)	0.0784 (2)	0.0372 (11)
C1	0.1808 (3)	0.5392 (8)	0.0749 (2)	0.0368 (14)

C2	0.1436 (3)	0.6216 (7)	0.1526 (3)	0.0340 (14)
C3	0.1835 (3)	0.4990 (8)	0.2376 (3)	0.0398 (16)
C4	0.2981 (3)	0.1674 (9)	0.3335 (3)	0.0475 (17)
C5	0.3681 (3)	−0.0242 (10)	0.3370 (3)	0.0551 (17)
C6	0.3985 (3)	−0.0855 (9)	0.2554 (3)	0.0538 (17)
C7	0.3611 (3)	0.0351 (9)	0.1686 (3)	0.0427 (17)
C8	0.2875 (3)	0.2323 (8)	0.1643 (3)	0.0365 (12)
C9	0.2566 (3)	0.3003 (8)	0.2465 (3)	0.0369 (14)
C10	0.0635 (3)	0.8293 (8)	0.1397 (3)	0.0436 (16)
C11	0.3954 (3)	−0.0328 (10)	0.0817 (3)	0.0589 (17)
H1O	0.00970	0.73400	0.23830	0.0800*
H3	0.16230	0.54700	0.29100	0.0480*
H4	0.27790	0.20970	0.38810	0.0570*
H5	0.39560	−0.11390	0.39410	0.0660*
H6	0.44670	−0.21540	0.26010	0.0640*
H10A	0.08110	1.01170	0.11630	0.0520*
H10B	0.01230	0.75250	0.09200	0.0520*
H11A	0.44600	−0.16520	0.09810	0.0880*
H11B	0.41540	0.14190	0.05710	0.0880*
H11C	0.34680	−0.11840	0.03440	0.0880*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0614 (8)	0.0749 (9)	0.0457 (7)	0.0113 (7)	0.0170 (6)	0.0132 (6)
O1	0.060 (2)	0.0369 (17)	0.078 (2)	0.0016 (16)	0.0457 (18)	−0.0011 (16)
N1	0.042 (2)	0.035 (2)	0.0375 (19)	−0.0031 (18)	0.0153 (17)	−0.0004 (17)
C1	0.044 (3)	0.031 (2)	0.037 (2)	−0.007 (2)	0.013 (2)	−0.0008 (19)
C2	0.040 (3)	0.028 (2)	0.037 (2)	−0.005 (2)	0.015 (2)	−0.003 (2)
C3	0.044 (3)	0.043 (3)	0.039 (2)	−0.009 (2)	0.023 (2)	−0.006 (2)
C4	0.051 (3)	0.052 (3)	0.042 (3)	−0.010 (3)	0.016 (2)	0.000 (2)
C5	0.053 (3)	0.063 (3)	0.047 (3)	−0.004 (3)	0.007 (2)	0.012 (2)
C6	0.038 (3)	0.051 (3)	0.071 (3)	−0.001 (2)	0.010 (3)	0.011 (3)
C7	0.037 (3)	0.044 (3)	0.048 (3)	−0.006 (2)	0.012 (2)	0.002 (2)
C8	0.037 (2)	0.036 (2)	0.038 (2)	−0.007 (2)	0.012 (2)	−0.002 (2)
C9	0.043 (3)	0.036 (2)	0.034 (2)	−0.007 (2)	0.014 (2)	−0.003 (2)
C10	0.046 (3)	0.038 (2)	0.053 (3)	−0.004 (2)	0.024 (2)	−0.002 (2)
C11	0.050 (3)	0.069 (3)	0.063 (3)	0.010 (3)	0.024 (2)	−0.006 (3)

Geometric parameters (Å, º)

Cl1—C1	1.735 (3)	C7—C11	1.499 (6)
O1—C10	1.406 (5)	C7—C8	1.421 (6)
O1—H1O	0.8200	C8—C9	1.409 (6)
N1—C8	1.373 (5)	C3—H3	0.9300
N1—C1	1.307 (5)	C4—H4	0.9300
C1—C2	1.419 (6)	C5—H5	0.9300
C2—C10	1.514 (6)	C6—H6	0.9300

C2—C3	1.359 (6)	C10—H10A	0.9700
C3—C9	1.412 (6)	C10—H10B	0.9700
C4—C9	1.408 (6)	C11—H11A	0.9600
C4—C5	1.365 (6)	C11—H11B	0.9600
C5—C6	1.391 (6)	C11—H11C	0.9600
C6—C7	1.368 (6)		

C10—O1—H1O	110.00	O1—C10—C2	113.5 (3)
C1—N1—C8	117.8 (3)	C2—C3—H3	119.00
Cl1—C1—N1	116.2 (3)	C9—C3—H3	119.00
Cl1—C1—C2	117.9 (3)	C5—C4—H4	120.00
N1—C1—C2	126.0 (3)	C9—C4—H4	120.00
C1—C2—C3	115.7 (4)	C4—C5—H5	120.00
C1—C2—C10	121.3 (4)	C6—C5—H5	120.00
C3—C2—C10	122.9 (4)	C5—C6—H6	118.00
C2—C3—C9	121.4 (4)	C7—C6—H6	118.00
C5—C4—C9	119.4 (4)	O1—C10—H10A	109.00
C4—C5—C6	120.2 (4)	O1—C10—H10B	109.00
C5—C6—C7	123.4 (4)	C2—C10—H10A	109.00
C6—C7—C11	122.5 (4)	C2—C10—H10B	109.00
C8—C7—C11	120.9 (4)	H10A—C10—H10B	108.00
C6—C7—C8	116.6 (4)	C7—C11—H11A	109.00
N1—C8—C9	121.0 (4)	C7—C11—H11B	109.00
C7—C8—C9	120.8 (4)	C7—C11—H11C	109.00
N1—C8—C7	118.2 (4)	H11A—C11—H11B	109.00
C3—C9—C4	122.4 (4)	H11A—C11—H11C	109.00
C4—C9—C8	119.6 (4)	H11B—C11—H11C	110.00
C3—C9—C8	118.0 (4)		

C8—N1—C1—Cl1	−179.2 (3)	C9—C4—C5—C6	0.5 (7)
C8—N1—C1—C2	1.0 (6)	C5—C4—C9—C3	179.6 (4)
C1—N1—C8—C7	179.8 (4)	C5—C4—C9—C8	0.4 (6)
C1—N1—C8—C9	−1.5 (6)	C4—C5—C6—C7	−0.7 (7)
Cl1—C1—C2—C3	−179.7 (3)	C5—C6—C7—C8	0.0 (7)
Cl1—C1—C2—C10	1.3 (5)	C5—C6—C7—C11	179.6 (4)
N1—C1—C2—C3	0.1 (6)	C6—C7—C8—N1	179.6 (4)
N1—C1—C2—C10	−178.9 (4)	C6—C7—C8—C9	0.9 (6)
C1—C2—C3—C9	−0.7 (6)	C11—C7—C8—N1	0.0 (6)
C10—C2—C3—C9	178.3 (4)	C11—C7—C8—C9	−178.7 (4)
C1—C2—C10—O1	178.4 (3)	N1—C8—C9—C3	1.0 (6)
C3—C2—C10—O1	−0.6 (5)	N1—C8—C9—C4	−179.8 (4)
C2—C3—C9—C4	−179.1 (4)	C7—C8—C9—C3	179.7 (4)
C2—C3—C9—C8	0.1 (6)	C7—C8—C9—C4	−1.1 (6)

Hydrogen-bond geometry (Å, º)

Cg1 is a centroid of the N1/C1–C3/C8/C9 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*O*···O1^{i}	0.82	1.90	2.712 (4)	174
C10—H10*A*···*Cg*1^{ii}	0.97	2.75	3.557 (4)	141

Symmetry codes: (i) −*x*, *y*−1/2, −*z*+1/2; (ii) *x*, *y*+1, *z*.