Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

5-Chloroquinolin-8-yl furan-2-carboxylate

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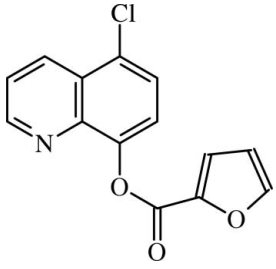
Received 22 February 2013; accepted 26 February 2013

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.043; wR factor = 0.119; data-to-parameter ratio = 14.2.

In the title compound, $C_{14}H_8ClNO_3$, the central ester CO_2 group is twisted away from the quinoline and furoyl rings by 57.46 (5) and 2.0 (1)°, respectively. In the crystal, molecules are linked by weak C—H···O interactions, forming chains in [001].

Related literature

For medicinal, antifungal, antibacterial, anticancer and luminiscent properties of the quinoline ring, see: Somvanshi *et al.* (2008), Biavatti *et al.* (2002), Towers *et al.* (1981), Shen *et al.* (1999) and Montes *et al.* (2006), respectively. For similar structures, see: Lei (2006; 2007). For hydrogen-bonding notation, see: Etter (1990); Nardelli (1995).



Experimental

Crystal data

$C_{14}H_8ClNO_3$
M_r = 273.66
Monoclinic, $P2_1/c$
a = 4.0714 (1) Å
b = 23.7463 (7) Å
c = 12.7698 (4) Å
β = 102.113 (1)°
V = 1207.11 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 295 K
0.35 × 0.09 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
4385 measured reflections
2440 independent reflections
1906 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.03
2440 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O2^{i}	0.93	2.47	3.371 (2)	162

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

RMF is grateful to the Spanish Research Council (CSIC) for the use of a free-of-charge licence to the Cambridge Structural Database. RMF also thanks the Universidad del Valle, Colombia, for partial financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2111).

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supporting information

Acta Cryst. (2013). E**69**, o501 [doi:10.1107/S1600536813005667]

5-Chloroquinolin-8-yl furan-2-carboxylate

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S1. Comment

The title compound, $C_{14}H_8ClNO_3$ [5-chloroquinolin-8-yl-furan-2-carboxylate] (I), is part of a series of studies on the structural properties of the quinoline fragment developed by our research group. The quinoline ring exhibits a key factor responsible for a wide range of medicinal (Somvanshi *et al.*, 2008), antifungal (Biavatti *et al.*, 2002) and antibacterial (Towers *et al.*, 1981) properties. The quinoline ring has been also used in anticancer studies (Shen *et al.*, 1999), as well as its derivatives have been exploited for their luminescent properties as organic light-emitting diodes (OLED) materials (Montes *et al.*, 2006). The molecular structure of (I) is shown in Fig. 1. Bond lengths and bond angles of (I) show marked similarity with other 8-Hydroxyquinoline benzoates reported in the literature such as 8-Quinolyl benzoate and 2-Methyl-quinolin-8-yl 2-nitrobenzoate (Lei, 2006 and 2007). The central ester moiety, C8/O1/C10/O2/C11, is essentially planar with a r.m.s deviation of fitted atoms of 0.007 Å. The ester group is twisted away from the quinoline and furoyl rings by 57.45 (5)° and 2.0 (1)°, respectively. The crystal packing shows no classical hydrogen bonds. The crystal packing is stabilized by weak C-H···O intermolecular interactions, forming C(6) chains along [001] (see Fig. 2; Etter, 1990). The C14 atom of the furoyl ring at (x,y,z) acts as a hydrogen-bond donor to carbonyl atom O2 at (x-1,-y+1/2,+z-1/2) (see Table 1; Nardelli, 1995).

S2. Experimental

The reagents and solvents for the synthesis were obtained from the Aldrich Chemical Co. and were used without additional purification. In a 100 ml round bottom flask 2-furoyl chloride (1.564 mmol, 0.204 g) and 5-chloro-8hidroxyquinoline (1.564 mmol, 0.260 g) in equimolar amounts were mixed. The mixture was left to reflux in 20 ml of acetonitrile in constant stirring for about two hours, adding small amounts of pyridine as catalyst. A colourless solid was obtained after leaving the solvent to evaporate. IR spectra were recorded on a FT—IR SHIMADZU IR-Affinity-1 spectrophotometer. Colourless crystals; m.p 389 (1) K. IR (KBr) 3127 cm^{-1}, 3097 cm^{-1} (aromatic C—H); 1743 cm^{-1} (ester C=O), 1299 cm^{-1} (ester C-O); 1588 cm^{-1}, 1495 cm^{-1}, 1392 cm^{-1} (amine C—N); 1467 cm^{-1} (furan C-O); 1181 cm^{-1} (C=C); 936 cm^{-1} (Cl-C).

S3. Refinement

All the H-atoms attached to C atoms were positioned at geometrically idealized positions and treated as riding with C—H= 0.93 Å and U_{iso}(H) = 1.2 U_{eq}(C).

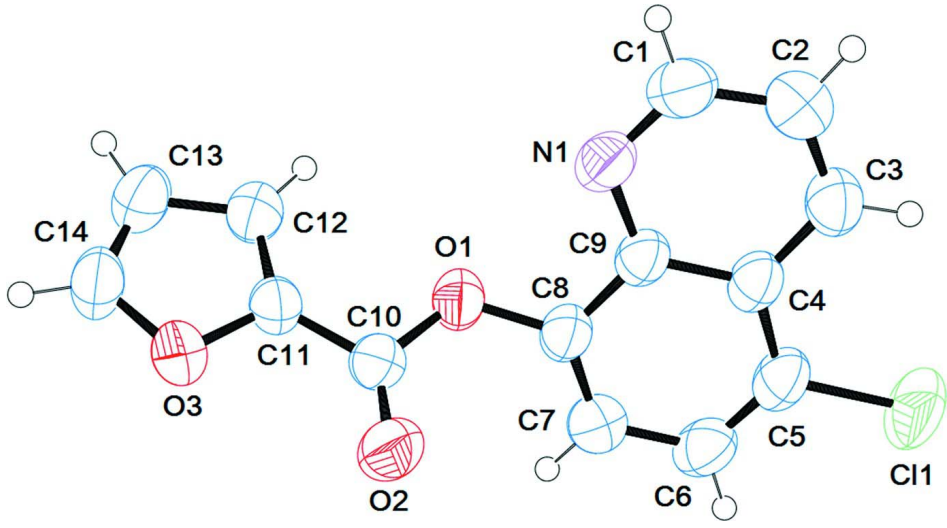

Figure 1

Molecular conformation and atom numbering scheme for the title compound (I) with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

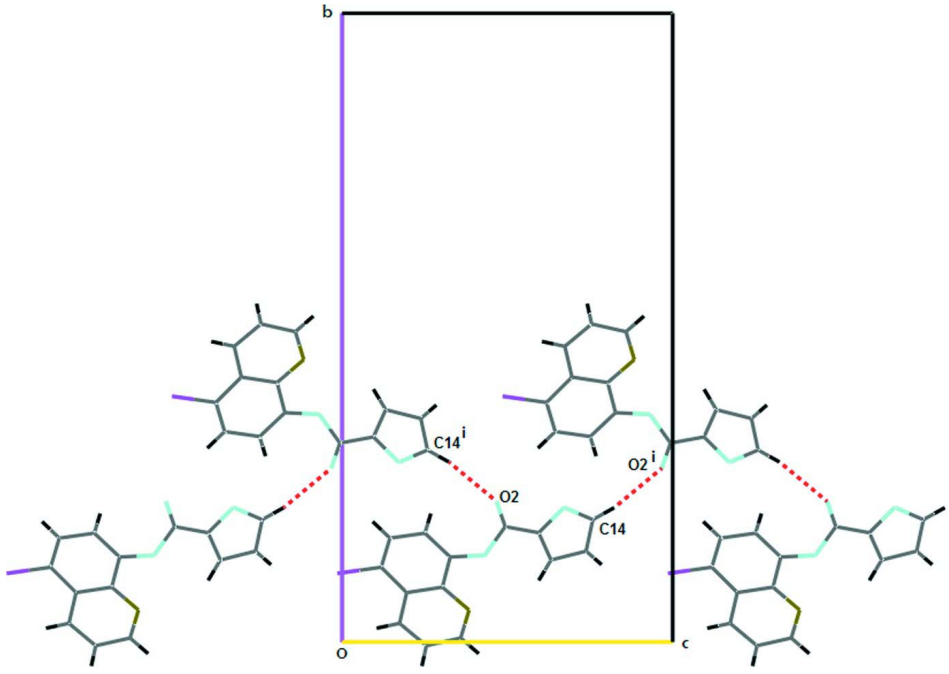

Figure 2

Part of the crystal structure of (I), showing the formation of helical chains which align along [001]. Symmetry code: (i) x-1,-y+1/2,+z-1/2.

5-Chloroquinolin-8-yl furan-2-carboxylate

Crystal data

$C_{14}H_8ClNO_3$
M_r = 273.66
Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc
a = 4.0714 (1) Å
b = 23.7463 (7) Å

c = 12.7698 (4) Å
β = 102.113 (1)°
V = 1207.11 (6) Å^3
Z = 4
F(000) = 560
D_x = 1.506 Mg m^{-3}
Melting point: 389(1) K

Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2589 reflections
θ = 3.1–26.3°
μ = 0.32 mm^{-1}
T = 295 K
Needle, colourless
0.35 × 0.09 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
CCD rotation images, thick slices scans
4385 measured reflections
2440 independent reflections

1906 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.3°, θ_{min} = 3.1°
h = −5→5
k = −29→27
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.119
S = 1.03
2440 reflections
172 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
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.2631P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *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	0.86765 (17)	0.10906 (3)	1.01429 (4)	0.0852 (3)
O3	−0.0985 (4)	0.21415 (5)	0.32844 (10)	0.0617 (4)
O2	0.3216 (4)	0.22368 (6)	0.53277 (11)	0.0735 (4)
O1	0.1366 (3)	0.13797 (5)	0.56894 (10)	0.0590 (4)
N1	0.5632 (4)	0.05097 (6)	0.61584 (11)	0.0518 (4)
C9	0.5359 (4)	0.08729 (7)	0.69653 (13)	0.0442 (4)
C3	0.9075 (5)	0.02976 (8)	0.82623 (15)	0.0578 (5)
H3	1.0231	0.0221	0.8956	0.069*
C4	0.7073 (4)	0.07857 (7)	0.80464 (13)	0.0470 (4)
C10	0.1468 (4)	0.18356 (7)	0.50701 (13)	0.0471 (4)

C8	0.3285 (5)	0.13513 (7)	0.67304 (14)	0.0491 (4)
C6	0.4679 (5)	0.16529 (8)	0.85564 (15)	0.0592 (5)
H6	0.4485	0.1917	0.9078	0.071*
C2	0.9304 (5)	−0.00590 (9)	0.74516 (17)	0.0630 (5)
H2	1.0611	−0.0383	0.7585	0.076*
C12	−0.2882 (5)	0.13064 (8)	0.36831 (15)	0.0540 (4)
H12	−0.3217	0.0982	0.4054	0.065*
C11	−0.0828 (4)	0.17374 (7)	0.40520 (13)	0.0456 (4)
C7	0.2944 (5)	0.17315 (8)	0.74910 (16)	0.0568 (5)
H7	0.1566	0.2044	0.7310	0.068*
C14	−0.3227 (6)	0.19455 (10)	0.24173 (16)	0.0668 (6)
H14	−0.3837	0.2136	0.1769	0.080*
C5	0.6638 (5)	0.11902 (8)	0.88183 (14)	0.0540 (5)
C1	0.7556 (5)	0.00645 (8)	0.64139 (16)	0.0592 (5)
H1	0.7767	−0.0184	0.5869	0.071*
C13	−0.4431 (5)	0.14454 (10)	0.26179 (16)	0.0654 (5)
H13	−0.5989	0.1229	0.2149	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1006 (5)	0.1148 (5)	0.0337 (3)	0.0015 (4)	−0.0007 (3)	−0.0047 (3)
O3	0.0868 (9)	0.0501 (7)	0.0449 (7)	0.0020 (6)	0.0064 (7)	0.0084 (5)
O2	0.1084 (11)	0.0582 (8)	0.0486 (8)	−0.0317 (8)	0.0048 (7)	0.0004 (6)
O1	0.0734 (8)	0.0500 (7)	0.0447 (7)	−0.0140 (6)	−0.0080 (6)	0.0094 (6)
N1	0.0647 (9)	0.0509 (8)	0.0395 (8)	−0.0130 (7)	0.0102 (7)	−0.0050 (6)
C9	0.0526 (10)	0.0451 (9)	0.0344 (8)	−0.0115 (7)	0.0079 (7)	0.0001 (7)
C3	0.0614 (11)	0.0620 (11)	0.0475 (10)	−0.0011 (9)	0.0056 (8)	0.0094 (9)
C4	0.0513 (10)	0.0520 (10)	0.0369 (8)	−0.0089 (8)	0.0077 (7)	0.0027 (7)
C10	0.0581 (10)	0.0434 (9)	0.0403 (9)	−0.0011 (8)	0.0115 (7)	0.0006 (7)
C8	0.0585 (10)	0.0470 (9)	0.0383 (9)	−0.0095 (8)	0.0023 (7)	0.0038 (7)
C6	0.0748 (13)	0.0603 (11)	0.0448 (10)	−0.0083 (10)	0.0175 (9)	−0.0107 (8)
C2	0.0687 (12)	0.0553 (11)	0.0659 (13)	0.0038 (9)	0.0160 (10)	0.0043 (9)
C12	0.0557 (10)	0.0539 (10)	0.0499 (10)	−0.0021 (8)	0.0051 (8)	0.0021 (8)
C11	0.0543 (10)	0.0435 (9)	0.0395 (9)	0.0061 (7)	0.0109 (7)	0.0039 (7)
C7	0.0650 (11)	0.0503 (10)	0.0543 (11)	−0.0005 (9)	0.0108 (9)	0.0003 (8)
C14	0.0805 (14)	0.0729 (14)	0.0418 (10)	0.0171 (11)	0.0008 (9)	0.0058 (9)
C5	0.0609 (11)	0.0663 (12)	0.0339 (9)	−0.0085 (9)	0.0080 (8)	−0.0027 (8)
C1	0.0717 (12)	0.0515 (10)	0.0564 (12)	−0.0082 (9)	0.0181 (9)	−0.0094 (9)
C13	0.0626 (12)	0.0755 (14)	0.0508 (11)	0.0014 (10)	−0.0047 (9)	−0.0035 (10)

Geometric parameters (Å, º)

Cl1—C5	1.7370 (18)	C4—C9	1.425 (2)
O1—C8	1.395 (2)	C5—C6	1.358 (3)
O1—C10	1.347 (2)	C6—C7	1.408 (3)
O2—C10	1.193 (2)	C6—H6	0.9300
O3—C11	1.364 (2)	C7—C8	1.355 (3)

O3—C14	1.361 (2)	C7—H7	0.9300
N1—C1	1.316 (2)	C8—C9	1.410 (2)
N1—C9	1.366 (2)	C10—C11	1.452 (2)
C1—C2	1.397 (3)	C11—C12	1.343 (2)
C1—H1	0.9300	C12—C13	1.413 (3)
C2—C3	1.356 (3)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.330 (3)
C3—C4	1.410 (3)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.414 (3)		

C14—O3—C11	105.45 (15)	C1—C2—H2	120.3
C10—O1—C8	121.21 (13)	C11—C12—C13	106.20 (17)
C1—N1—C9	117.31 (15)	C11—C12—H12	126.9
N1—C9—C8	119.22 (14)	C13—C12—H12	126.9
N1—C9—C4	122.55 (16)	C12—C11—O3	110.63 (15)
C8—C9—C4	118.23 (15)	C12—C11—C10	132.30 (16)
C2—C3—C4	119.58 (17)	O3—C11—C10	117.05 (15)
C2—C3—H3	120.2	C8—C7—C6	119.90 (18)
C4—C3—H3	120.2	C8—C7—H7	120.0
C3—C4—C5	125.02 (16)	C6—C7—H7	120.0
C3—C4—C9	117.01 (16)	C13—C14—O3	111.11 (17)
C5—C4—C9	117.96 (16)	C13—C14—H14	124.4
O2—C10—O1	124.77 (16)	O3—C14—H14	124.4
O2—C10—C11	127.56 (16)	C6—C5—C4	122.09 (17)
O1—C10—C11	107.65 (14)	C6—C5—Cl1	119.07 (15)
C7—C8—O1	122.00 (17)	C4—C5—Cl1	118.83 (15)
C7—C8—C9	122.11 (16)	N1—C1—C2	124.20 (18)
O1—C8—C9	115.62 (15)	N1—C1—H1	117.9
C5—C6—C7	119.68 (17)	C2—C1—H1	117.9
C5—C6—H6	120.2	C14—C13—C12	106.60 (18)
C7—C6—H6	120.2	C14—C13—H13	126.7
C3—C2—C1	119.34 (19)	C12—C13—H13	126.7
C3—C2—H2	120.3		

C1—N1—C9—C8	−179.10 (16)	C14—O3—C11—C10	178.79 (16)
C1—N1—C9—C4	0.3 (2)	O2—C10—C11—C12	179.9 (2)
C2—C3—C4—C5	−179.79 (18)	O1—C10—C11—C12	1.4 (3)
C2—C3—C4—C9	0.4 (3)	O2—C10—C11—O3	1.4 (3)
N1—C9—C4—C3	−0.7 (2)	O1—C10—C11—O3	−177.05 (15)
C8—C9—C4—C3	178.71 (15)	O1—C8—C7—C6	173.41 (16)
N1—C9—C4—C5	179.51 (16)	C9—C8—C7—C6	−0.4 (3)
C8—C9—C4—C5	−1.1 (2)	C5—C6—C7—C8	−1.2 (3)
C8—O1—C10—O2	2.3 (3)	C11—O3—C14—C13	−0.1 (2)
C8—O1—C10—C11	−179.13 (15)	C7—C6—C5—C4	1.6 (3)
C10—O1—C8—C7	59.4 (2)	C7—C6—C5—Cl1	−178.39 (14)
C10—O1—C8—C9	−126.42 (17)	C3—C4—C5—C6	179.78 (18)
N1—C9—C8—C7	−179.07 (17)	C9—C4—C5—C6	−0.4 (3)

C4—C9—C8—C7	1.5 (3)	C3—C4—C5—Cl1	−0.2 (3)
N1—C9—C8—O1	6.8 (2)	C9—C4—C5—Cl1	179.55 (12)
C4—C9—C8—O1	−172.65 (14)	C9—N1—C1—C2	0.4 (3)
C4—C3—C2—C1	0.2 (3)	C3—C2—C1—N1	−0.6 (3)
C13—C12—C11—O3	0.0 (2)	O3—C14—C13—C12	0.1 (2)
C13—C12—C11—C10	−178.50 (18)	C11—C12—C13—C14	−0.1 (2)
C14—O3—C11—C12	0.0 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O2^{i}	0.93	2.47	3.371 (2)	162

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