Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Chlorophenyl)-4-hydroxyfuran-2(5*H*)-one

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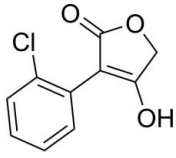
Received 8 November 2011; accepted 15 November 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.108; data-to-parameter ratio = 17.0.

In the title molecule, $C_{10}H_7ClO_3$, the butyrolactone core, a furan-2(5*H*)-one, forms a dihedral angle of 59.21 (5)° with the benzene ring. In the crystal, two types of hydrogen bonds (O—H···O and C—H···Cl) link molecules into infinite chains along the *b* axis. π–π contacts [centroid–centroid distances = 3.6359 (10) and 3.8776 (11) Å] link the chains into a three-dimensional network.

Related literature

For the antibacterial activity of furanones, see: Xiao *et al.* (2011). For related structures, see: Peng *et al.* (2011); Xiao *et al.* (2010).



Experimental

Crystal data

$C_{10}H_7ClO_3$
M_r = 210.61
Monoclinic, $P2_1/c$
a = 9.9699 (15) Å
b = 11.8308 (18) Å
c = 8.1562 (12) Å
β = 104.898 (2)°
V = 929.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.39 mm^{-1}
T = 296 K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.893, T_{max} = 0.927
7259 measured reflections
2240 independent reflections
2037 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.108
S = 1.12
2240 reflections
132 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O1^{i}	0.82 (3)	1.80 (3)	2.6182 (16)	170 (3)
C9—H9B···Cl1^{i}	0.97	2.77	3.7126 (16)	165

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The work was financed by the Planned Science and Technology Project of Hunan Province, China (grant No. 2011 F J3056), the Key Laboratory of Plant Resources Conservation and Utilization (Jishou University), College of Hunan Province (grant No. JSK201106) and Hunan Provincial Natural Science Foundation of China (grant No. 11 J J3113).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2483).

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supporting information

Acta Cryst. (2011). E**67**, o3428 [https://doi.org/10.1107/S1600536811048641]

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S1. Comment

Recently, we have reported the antibacterial activities of a few *γ*-butyrolactones (furanones) (Xiao *et al.*, 2011). As a part of our ongoing studies of *γ*-butyrolactones (Xiao *et al.*, 2010), we herein report the crystal structure of the title compound.

In the title compound (Fig. 1), the butyrolactone moiety makes a dihedral angle of 59.21 (5) ° with the benzene ring. Relatively strong intermolecular hydrogen bonds (O—H···O) link molecules into an infinite chain running along the *b* axis, which is further consolidated by weak intermolecular C—H···Cl interactions. There are *π*–*π* contacts between benzene rings and butyrolactone rings with centroid–centroid distances 3.6359 (10) and 3.8776 (11) Å, respectively (Fig. 2). The molecular dimensions in the title molecule agree very well with the corresponding molecular dimensions reported in a few similar structures (Peng *et al.*, 2011; Xiao *et al.*, 2010).

S2. Experimental

A dropwise solution of 2-ethoxy-2-oxoethyl 2-(2-chlorophenyl)acetate (1.03 g, 4 mmol) in dry THF was added to a suspension of NaH in dry THF in an ice cold bath. The stirring was maintained at room temperature for 6 h. Water was added and the solution was extracted twice with ethyl ether. The aqueous phase was cooled to 273 K and then acidified with concentrated hydrochloric acid to give a solid precipitate. The title compound thus obtained was crystallized from ethanol-water (2:1) to give the colorless blocks suitable for single-crystal structure determination.

S3. Refinement

The H-atoms bonded to C-atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 and 0.97 Å for aryl and methylene type H atoms, respectively, with U_{iso}(H) = 1.2 U_{eq}(C). The hydroxyl H atom was located from a difference Fourier map and was allowed to refine freely.

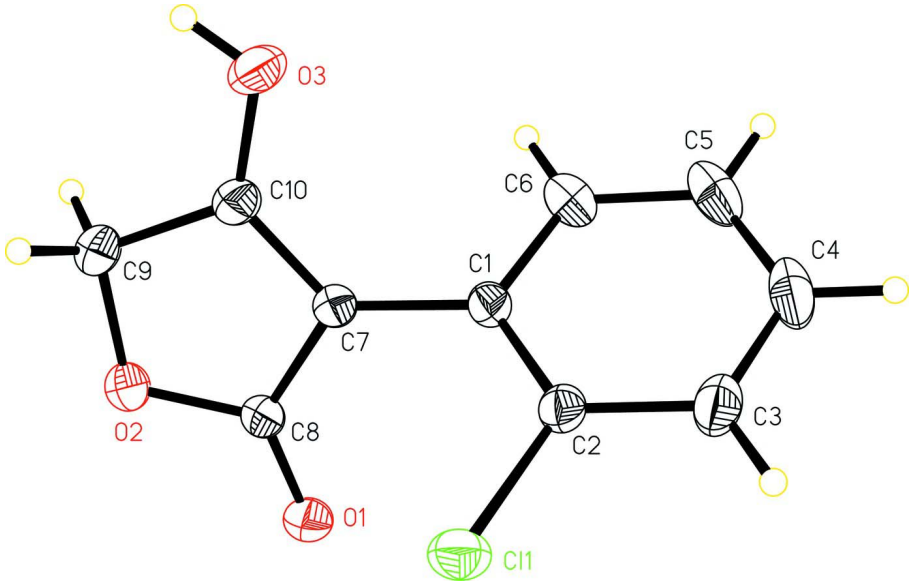

Figure 1

Molecular structure of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

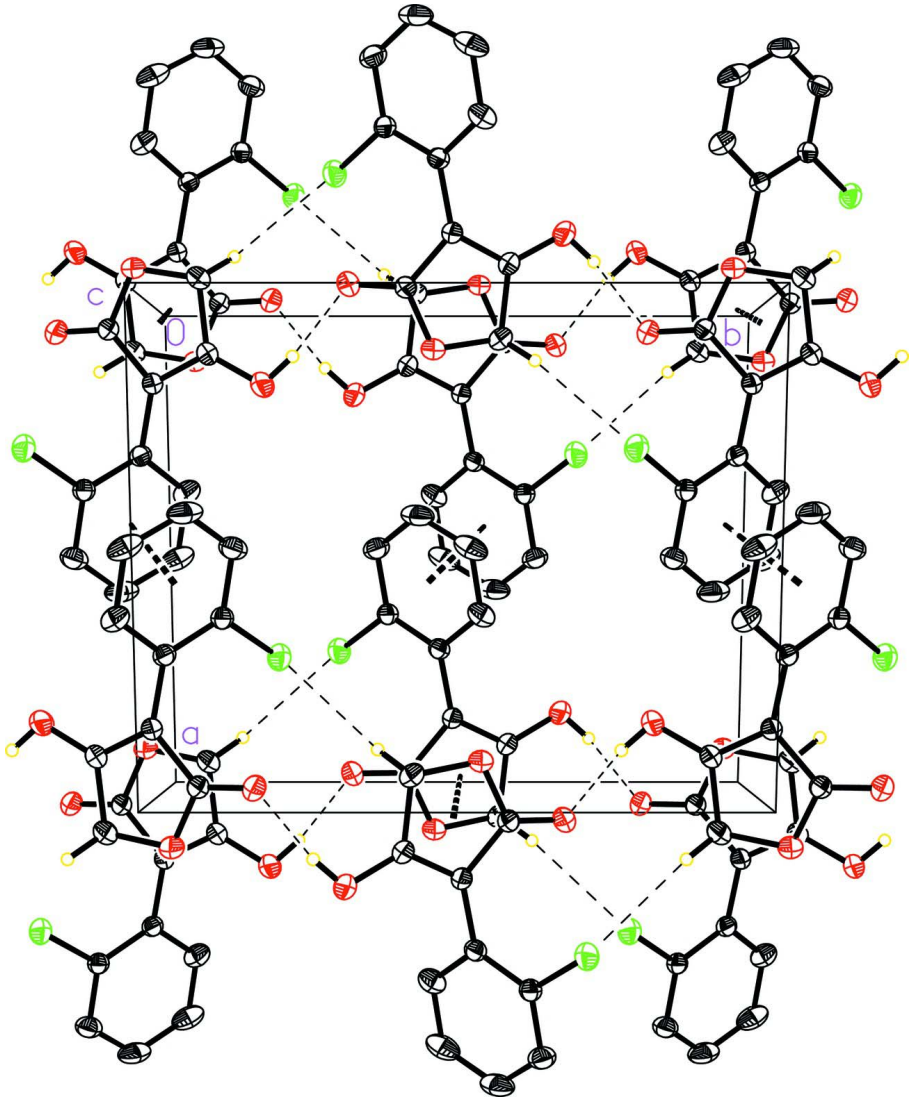

Figure 2

A unit cell packing diagram of the title compound showing a three-dimensional network built through intermolecular hydrogen bonds and π–π contacts.

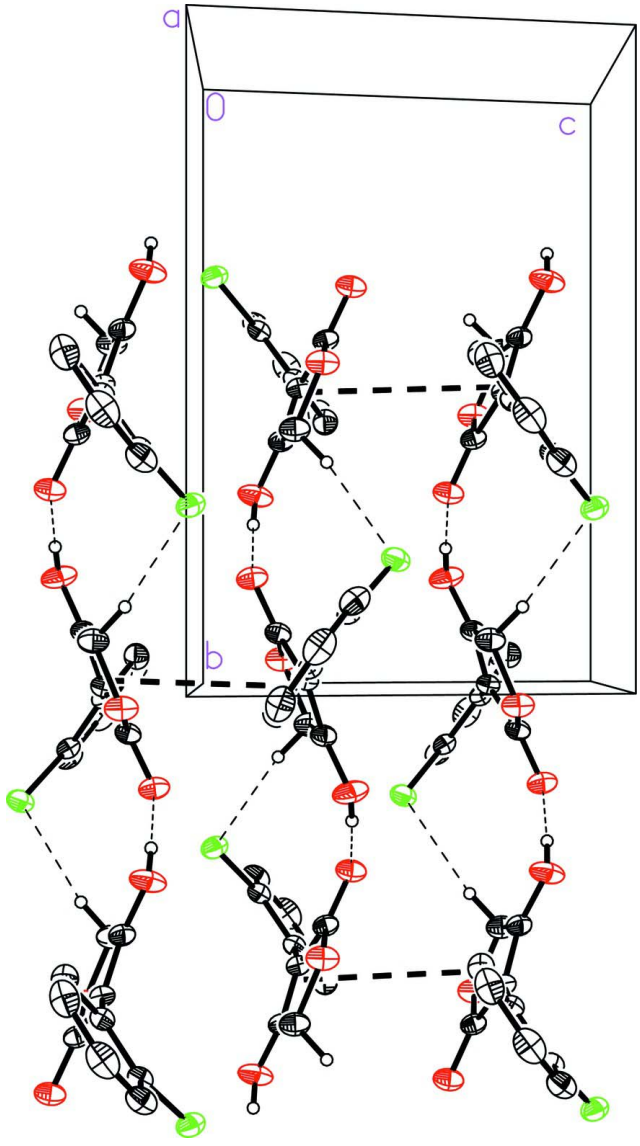

Figure 3

A unit cell packing diagram of the title compound

3-(2-Chlorophenyl)-4-hydroxyfuran-2(5*H*)-one

Crystal data

$C_{10}H_7ClO_3$
$M_r = 210.61$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 9.9699\ (15)$ Å
$b = 11.8308\ (18)$ Å
$c = 8.1562\ (12)$ Å
$\beta = 104.898\ (2)°$
$V = 929.7\ (2)$ Å^3
$Z = 4$

$F(000) = 432$
$D_x = 1.505$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2125 reflections
$\theta = 2.7–27.8°$
$\mu = 0.39$ mm^{-1}
$T = 296$ K
Block, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scan
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.893, T_{max} = 0.927
7259 measured reflections
2240 independent reflections
2037 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 28.0°, θ_{min} = 2.1°
h = −13→10
k = −15→15
l = −10→10

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.108
S = 1.12
2240 reflections
132 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0607P)^2 + 0.1971P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.021 (4)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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}
C1	0.70093 (13)	0.46964 (11)	0.22948 (16)	0.0334 (3)
C2	0.62894 (13)	0.38058 (11)	0.13494 (17)	0.0350 (3)
C3	0.48970 (15)	0.36149 (14)	0.1245 (2)	0.0475 (4)
H3A	0.4435	0.3010	0.0617	0.057*
C4	0.42063 (16)	0.43319 (17)	0.2082 (2)	0.0567 (4)
H4	0.3274	0.4206	0.2022	0.068*
C5	0.48850 (17)	0.52330 (17)	0.3006 (2)	0.0556 (4)
H5	0.4408	0.5719	0.3553	0.067*
C6	0.62747 (16)	0.54126 (14)	0.3117 (2)	0.0455 (3)
H6	0.6729	0.6019	0.3748	0.055*
C7	0.84833 (13)	0.49225 (10)	0.23989 (17)	0.0337 (3)
C8	0.96157 (13)	0.41569 (11)	0.31055 (18)	0.0365 (3)
C9	1.05960 (15)	0.57272 (12)	0.2315 (2)	0.0459 (3)
H9A	1.0901	0.5790	0.1281	0.055*
H9B	1.1076	0.6290	0.3119	0.055*

C10	0.90647 (14)	0.58691 (11)	0.19598 (18)	0.0380 (3)
Cl1	0.71082 (4)	0.29321 (3)	0.01933 (5)	0.04628 (15)
H3	0.897 (3)	0.730 (2)	0.125 (3)	0.080 (7)*
O1	0.95949 (11)	0.32284 (8)	0.37570 (15)	0.0465 (3)
O2	1.08432 (10)	0.46088 (9)	0.30186 (16)	0.0482 (3)
O3	0.84132 (12)	0.67963 (10)	0.12899 (18)	0.0564 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0298 (6)	0.0325 (6)	0.0387 (6)	0.0021 (4)	0.0102 (5)	0.0046 (5)
C2	0.0319 (6)	0.0325 (6)	0.0400 (6)	0.0003 (5)	0.0082 (5)	0.0070 (5)
C3	0.0328 (7)	0.0490 (8)	0.0568 (9)	−0.0059 (6)	0.0046 (6)	0.0136 (7)
C4	0.0296 (7)	0.0776 (12)	0.0647 (10)	0.0058 (7)	0.0156 (7)	0.0213 (9)
C5	0.0430 (8)	0.0773 (12)	0.0514 (9)	0.0217 (8)	0.0208 (7)	0.0107 (8)
C6	0.0417 (7)	0.0505 (8)	0.0454 (7)	0.0105 (6)	0.0128 (6)	−0.0012 (6)
C7	0.0306 (6)	0.0290 (6)	0.0419 (6)	−0.0011 (4)	0.0101 (5)	−0.0033 (5)
C8	0.0318 (6)	0.0314 (6)	0.0470 (7)	0.0004 (5)	0.0117 (5)	−0.0048 (5)
C9	0.0356 (7)	0.0384 (7)	0.0648 (9)	−0.0071 (5)	0.0149 (6)	−0.0014 (6)
C10	0.0345 (6)	0.0311 (6)	0.0469 (7)	−0.0040 (5)	0.0080 (5)	−0.0031 (5)
Cl1	0.0483 (2)	0.0362 (2)	0.0521 (2)	0.00220 (13)	0.00863 (16)	−0.00722 (13)
O1	0.0408 (5)	0.0334 (5)	0.0656 (7)	0.0049 (4)	0.0140 (5)	0.0054 (4)
O2	0.0304 (5)	0.0397 (5)	0.0752 (7)	0.0007 (4)	0.0146 (5)	0.0014 (5)
O3	0.0410 (6)	0.0344 (5)	0.0876 (9)	−0.0053 (4)	0.0056 (6)	0.0141 (6)

Geometric parameters (Å, º)

C1—C2	1.3912 (18)	C6—H6	0.9300
C1—C6	1.3987 (19)	C7—C10	1.3510 (18)
C1—C7	1.4745 (17)	C7—C8	1.4465 (17)
C2—C3	1.3873 (19)	C8—O1	1.2228 (17)
C2—Cl1	1.7377 (14)	C8—O2	1.3539 (16)
C3—C4	1.379 (3)	C9—O2	1.4382 (18)
C3—H3A	0.9300	C9—C10	1.488 (2)
C4—C5	1.378 (3)	C9—H9A	0.9700
C4—H4	0.9300	C9—H9B	0.9700
C5—C6	1.381 (2)	C10—O3	1.3195 (17)
C5—H5	0.9300	O3—H3	0.82 (3)
C2—C1—C6	117.73 (12)	C10—C7—C8	106.29 (11)
C2—C1—C7	122.26 (11)	C10—C7—C1	128.63 (12)
C6—C1—C7	119.97 (12)	C8—C7—C1	125.00 (11)
C3—C2—C1	121.53 (13)	O1—C8—O2	119.61 (12)
C3—C2—Cl1	118.17 (11)	O1—C8—C7	129.56 (12)
C1—C2—Cl1	120.26 (10)	O2—C8—C7	110.81 (11)
C4—C3—C2	119.25 (15)	O2—C9—C10	104.08 (11)
C4—C3—H3A	120.4	O2—C9—H9A	110.9
C2—C3—H3A	120.4	C10—C9—H9A	110.9

C5—C4—C3	120.60 (14)	O2—C9—H9B	110.9
C5—C4—H4	119.7	C10—C9—H9B	110.9
C3—C4—H4	119.7	H9A—C9—H9B	109.0
C4—C5—C6	119.86 (15)	O3—C10—C7	126.86 (13)
C4—C5—H5	120.1	O3—C10—C9	123.04 (12)
C6—C5—H5	120.1	C7—C10—C9	110.09 (12)
C5—C6—C1	121.02 (16)	C8—O2—C9	108.65 (10)
C5—C6—H6	119.5	C10—O3—H3	111.0 (18)
C1—C6—H6	119.5		

C6—C1—C2—C3	−1.21 (19)	C6—C1—C7—C8	119.84 (15)
C7—C1—C2—C3	−179.04 (12)	C10—C7—C8—O1	175.41 (15)
C6—C1—C2—Cl1	176.21 (10)	C1—C7—C8—O1	−1.6 (2)
C7—C1—C2—Cl1	−1.61 (17)	C10—C7—C8—O2	−2.92 (16)
C1—C2—C3—C4	0.7 (2)	C1—C7—C8—O2	−179.92 (12)
Cl1—C2—C3—C4	−176.74 (12)	C8—C7—C10—O3	−178.86 (15)
C2—C3—C4—C5	0.4 (2)	C1—C7—C10—O3	−2.0 (2)
C3—C4—C5—C6	−0.9 (3)	C8—C7—C10—C9	2.03 (16)
C4—C5—C6—C1	0.4 (2)	C1—C7—C10—C9	178.90 (13)
C2—C1—C6—C5	0.6 (2)	O2—C9—C10—O3	−179.72 (14)
C7—C1—C6—C5	178.52 (14)	O2—C9—C10—C7	−0.57 (17)
C2—C1—C7—C10	121.29 (16)	O1—C8—O2—C9	−175.94 (13)
C6—C1—C7—C10	−56.5 (2)	C7—C8—O2—C9	2.58 (16)
C2—C1—C7—C8	−62.39 (19)	C10—C9—O2—C8	−1.25 (16)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1^{i}	0.82 (3)	1.80 (3)	2.6182 (16)	170 (3)
C9—H9*B*···Cl1^{i}	0.97	2.77	3.7126 (16)	165

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