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1-(1-Benzofuran-2-yl)-2-chloroethanone

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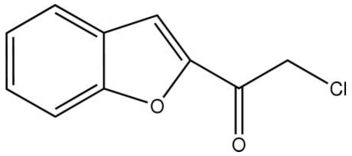
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.086; wR factor = 0.165; data-to-parameter ratio = 23.1.

The title compound, $C_{10}H_7ClO_2$, was synthesized from 1-benzofuran-2-ylethanone by chlorination with thionyl chloride. The benzofuran ring system and the carbonyl group are coplanar. The carbonyl group is in a *syn* position relative to both the O atom of the benzofuran ring and the Cl atom. C—H⋯O contacts are found between the methylene group and carbonyl O atom. Molecules related by a centre of symmetry are involved in π–π interactions, with distances between the centroids of the furan rings of 3.785 (3) Å.

Related literature

For related literature, see: Arıcı *et al.* (2004); Bachechi *et al.* (1988); Fothergill *et al.* (1977); Gareth (2001); Ocak Ískeleli *et al.* (2005); Narimatsu *et al.* (2003); Tanis *et al.* (2006); Thiruvalluvar *et al.* (2003); Weerawarna *et al.* (1991); Zaidlewicz *et al.* (2005).



Experimental

Crystal data

$C_{10}H_7ClO_2$
M_r = 194.61
Orthorhombic, *Pbca*
a = 9.550 (2) Å
b = 10.303 (2) Å
c = 17.695 (4) Å
V = 1741.1 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.40 mm^{-1}
T = 293 (2) K
0.34 × 0.14 × 0.08 mm

Data collection

Oxford Diffraction Sapphire CCD diffractometer
Absorption correction: numerical (*CrysAlis RED*; Oxford Diffraction, 2000)
$T_{\min}$ = 0.876, $T_{\max}$ = 0.968
16159 measured reflections
2726 independent reflections
1768 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.086
$wR(F^2)$ = 0.165
S = 1.24
2726 reflections
118 parameters
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.28 e Å^{-3}
$\Delta\rho_{\min}$ = −0.26 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
C9—H9B⋯O2$^{\rm i}$	0.97	2.49	3.238 (3)	134

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2000); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *CIFTAB* in *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2118).

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supplementary materials

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1-(1-Benzofuran-2-yl)-2-chloroethanone

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Comment

Aryl-2-chloroethanone and alkyl-2-chloroethanons are precursors of appropriate beta-amino-alfa-aryl (or alkyl) ethanols (Zaidlewicz *et al.*, 2005; Tanis *et al.*, 2006). These compounds containing the amino function exhibit the pharmacological activity. Many beta-amine arylethanol derivatives such as albuterol, isoproterenol, sotalol and terbutaline are well known beta-blockers or agonists and used in treatment of asthma, glaucoma, and cardiovascular disease (Gareth, 2001). All of them are nonselective beta-adrenoreceptor blocking agents comparable to propranolol (Weerawarna *et al.*, 1991; Fothergill *et al.*, 1977). Aromatic beta-aminoalcohols are also widely used as substrates in studies of the oxidation in liver by cytochrome P450 enzymes (Narimatsu *et al.*, 2003). Furthermore, many compounds mentioned above show an anti-arrythmic properties. Developing methods of their enantioselective synthesis is of particular importance.

We have found that crystal structure of the title compound is not known yet, although it is a well known substrate for the synthesis of benzofuran derivatives revealing different biological activity. Therefore, the aim of the study was to determine its molecular and crystal structures.

The molecule is planar with the dihedral angle of 1.9 (2) ^{o} between the best planes of benzofuran ring system and C2—C8—O2—C9 group containing carbonyl moiety. The chloromethylene moiety is almost co-planar with the ring system: the C2—C8—C9—Cl1 torsion angle is −175.8 (2) ^{o}, with the r.m.s. deviation of Cl1 from that plane of 0.079 (4) Å. The carbonyl O2 is in *syn* position relative to benzofuran O1, the O1—C2—C8—O2 torsion angle is 1.6 (4) ^{o}. The chlorine atom is positioned in *syn* orientation relative to carbonyl O2, with the O2—C8—C9—Cl1 torsion angle 4.7 (4) ^{o}. The valence geometry of the investigated compound is similar to that found for unsubstitituted compounds at position 3. In the reported structure the O1—C2 distance is 1.385 (3) Å and it is similar to 1.385 Å found in 2-acetylbenzo(*b*)furan (Thiruvalluvar *et al.*, 2003). However, the substituted compounds: [2-acetyl-3-(benzoylamino)-1-benzofuran (Ocak Ískeleli *et al.*, 2005), 2-acetyl-3-aminobenzofuran (Bachechi *et al.*, 1988), and 1-(3-amino-1-benzofuran-2-yl)-2-mesitylethanone (Arıcı *et al.*, 2004) reveal somewhat longer bond distances of 1.403–1.411 Å.

The packing analysis revealed that each molecule forms a pair of intermolecular C—H···O contact of 3.238 (3) Å along the *b* axis involving its C9—H methylene group and carbonyl oxygen, the C9···O2 ($0.5 - x$, $1/2 + y$, z). The packing interactions are completed by stacking of the ring systems of the molecules related by a centre of inversion ($1 - x$, $1 - y$, $-z$). Interaction π···π between adjacent molecules is characterized by distance between centroids of the furane moieties of 3.785 (3) Å. In these dimers anti-parallel orientation of molecules occurs.

Experimental

The title compound, 1-(benzofuran-2-yl)-2-chloroethanone, was synthesized from 1-benzofuran-2-ylethanone by chlorination with thionyl chloride in the carbon tetrachloride solution. Crystals suitable for the diffraction experiment were obtained by slow evaporation from the ethanol solution. Structure was solved with the direct methods and refined using *SHELX98* package (Sheldrick, 1997).

Refinement

Hydrogen atoms were put in the calculated positions and constrained during refinement (C—H 0.98 Å, aromatic C—H 0.93 Å, U fixed at 0.080 Å^2).

Figures

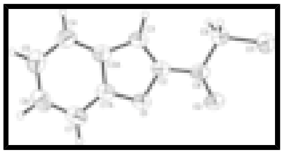

Fig. 1. A view of (I) with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

1-(1-Benzofuran-2-yl)-2-chloroethanone

Crystal data

$C_{10}H_7ClO_2$	F_{000} = 800
M_r = 194.61	D_x = 1.485 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P2ac2ab	Cell parameters from 2172 reflections
a = 9.550 (2) Å	θ = 3.1–31.4°
b = 10.303 (2) Å	μ = 0.40 mm^{-1}
c = 17.695 (4) Å	*T* = 293 (2) K
V = 1741.1 (6) Å^3	Plate, colorless
Z = 8	0.34 × 0.14 × 0.08 mm

Data collection

Oxford Diffraction Sapphire CCD diffractometer	2726 independent reflections
Radiation source: fine-focus sealed tube	1768 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.074
T = 293(2) K	θ_{max} = 31.4°
θ/2θ scans	θ_{min} = 3.1°
Absorption correction: numerical (CrysAlis RED; Oxford Diffraction, 2000)	$h = -13\rightarrow13$
T_{min} = 0.876, T_{max} = 0.968	$k = -14\rightarrow13$
16159 measured reflections	$l = -25\rightarrow23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.086$	H-atom parameters constrained
$wR(F^2) = 0.165$	$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.24$	$(\Delta/\sigma)_{max} = 0.003$
2726 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
118 parameters	$\Delta\rho_{min} = -0.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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*	$U_{iso}*/U_{eq}$
C2	0.3196 (3)	0.4735 (2)	−0.04559 (15)	0.0381 (6)
O1	0.3670 (2)	0.35910 (16)	−0.07774 (10)	0.0438 (5)
C3	0.3858 (3)	0.5771 (2)	−0.07517 (15)	0.0397 (6)
H2A	0.3715	0.6636	−0.0623	0.048*
C3A	0.4825 (3)	0.5288 (3)	−0.13015 (15)	0.0394 (6)
C4	0.5801 (3)	0.5831 (3)	−0.17913 (16)	0.0512 (8)
H4A	0.5930	0.6726	−0.1811	0.061*
C5	0.6573 (3)	0.5017 (3)	−0.22456 (17)	0.0556 (8)
H5A	0.7237	0.5364	−0.2573	0.067*
C6	0.6373 (3)	0.3680 (3)	−0.22217 (17)	0.0552 (8)
H6A	0.6900	0.3153	−0.2540	0.066*
C7	0.5418 (3)	0.3114 (3)	−0.17416 (16)	0.0499 (7)
H7A	0.5291	0.2220	−0.1722	0.060*
C7A	0.4662 (3)	0.3948 (3)	−0.12934 (14)	0.0395 (6)
O2	0.1674 (2)	0.35466 (18)	0.03153 (11)	0.0526 (6)
C8	0.2114 (3)	0.4601 (2)	0.01174 (15)	0.0393 (6)
C9	0.1580 (3)	0.5860 (3)	0.04366 (17)	0.0456 (7)
H9A	0.1140	0.6356	0.0036	0.055*
H9B	0.2365	0.6362	0.0626	0.055*
Cl1	0.03617 (8)	0.56222 (7)	0.11742 (4)	0.0546 (3)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C2	0.0427 (15)	0.0291 (13)	0.0425 (15)	0.0002 (11)	−0.0063 (12)	−0.0020 (12)
O1	0.0514 (12)	0.0303 (10)	0.0497 (12)	0.0004 (8)	0.0019 (9)	−0.0016 (9)
C3	0.0428 (16)	0.0306 (13)	0.0456 (16)	0.0018 (11)	−0.0027 (13)	−0.0018 (12)
C3A	0.0404 (16)	0.0355 (14)	0.0422 (16)	0.0013 (11)	−0.0085 (12)	0.0007 (12)
C4	0.056 (2)	0.0460 (17)	0.0511 (18)	−0.0035 (14)	0.0006 (15)	0.0045 (14)
C5	0.052 (2)	0.068 (2)	0.0468 (18)	0.0014 (15)	0.0039 (15)	0.0052 (16)
C6	0.061 (2)	0.064 (2)	0.0412 (17)	0.0169 (16)	−0.0033 (16)	−0.0043 (16)
C7	0.0599 (19)	0.0405 (16)	0.0494 (17)	0.0079 (14)	−0.0064 (15)	−0.0051 (14)
C7A	0.0426 (16)	0.0373 (14)	0.0387 (15)	0.0014 (12)	−0.0059 (13)	−0.0007 (11)
O2	0.0625 (14)	0.0335 (10)	0.0619 (14)	−0.0017 (9)	0.0071 (10)	0.0069 (10)
C8	0.0419 (16)	0.0326 (14)	0.0432 (15)	0.0005 (12)	−0.0102 (12)	0.0014 (12)
C9	0.0459 (17)	0.0372 (15)	0.0538 (18)	−0.0026 (12)	0.0055 (13)	−0.0012 (13)
Cl1	0.0539 (5)	0.0548 (5)	0.0549 (5)	0.0004 (3)	0.0070 (4)	−0.0025 (4)

Geometric parameters (Å, °)

C2—C3	1.346 (4)	C5—H5A	0.9300
C2—O1	1.385 (3)	C6—C7	1.376 (4)
C2—C8	1.454 (4)	C6—H6A	0.9300
O1—C7A	1.366 (3)	C7—C7A	1.374 (4)
C3—C3A	1.431 (4)	C7—H7A	0.9300
C3—H2A	0.9300	O2—C8	1.216 (3)
C3A—C7A	1.389 (4)	C8—C9	1.504 (4)
C3A—C4	1.391 (4)	C9—Cl1	1.766 (3)
C4—C5	1.376 (4)	C9—H9A	0.9700
C4—H4A	0.9300	C9—H9B	0.9700
C5—C6	1.391 (5)		
C3—C2—O1	111.2 (2)	C7—C6—H6A	119.0
C3—C2—C8	132.9 (2)	C5—C6—H6A	119.0
O1—C2—C8	115.9 (2)	C7A—C7—C6	116.1 (3)
C7A—O1—C2	105.79 (19)	C7A—C7—H7A	122.0
C2—C3—C3A	107.0 (2)	C6—C7—H7A	122.0
C2—C3—H2A	126.5	O1—C7A—C7	125.6 (3)
C3A—C3—H2A	126.5	O1—C7A—C3A	110.6 (2)
C7A—C3A—C4	118.8 (3)	C7—C7A—C3A	123.8 (3)
C7A—C3A—C3	105.4 (2)	O2—C8—C2	122.1 (2)
C4—C3A—C3	135.7 (3)	O2—C8—C9	123.0 (3)
C5—C4—C3A	118.5 (3)	C2—C8—C9	114.9 (2)
C5—C4—H4A	120.7	C8—C9—Cl1	112.41 (19)
C3A—C4—H4A	120.7	C8—C9—H9A	109.1
C4—C5—C6	120.8 (3)	Cl1—C9—H9A	109.1
C4—C5—H5A	119.6	C8—C9—H9B	109.1
C6—C5—H5A	119.6	Cl1—C9—H9B	109.1
C7—C6—C5	122.0 (3)	H9A—C9—H9B	107.9

C3—C2—O1—C7A	−0.2 (3)	C6—C7—C7A—O1	−179.7 (2)
C8—C2—O1—C7A	179.8 (2)	C6—C7—C7A—C3A	−0.5 (4)
O1—C2—C3—C3A	0.1 (3)	C4—C3A—C7A—O1	179.6 (2)
C8—C2—C3—C3A	−179.9 (3)	C3—C3A—C7A—O1	−0.2 (3)
C2—C3—C3A—C7A	0.0 (3)	C4—C3A—C7A—C7	0.3 (4)
C2—C3—C3A—C4	−179.7 (3)	C3—C3A—C7A—C7	−179.5 (3)
C7A—C3A—C4—C5	−0.4 (4)	C3—C2—C8—O2	−178.4 (3)
C3—C3A—C4—C5	179.3 (3)	O1—C2—C8—O2	1.6 (4)
C3A—C4—C5—C6	0.7 (4)	C3—C2—C8—C9	2.1 (4)
C4—C5—C6—C7	−0.8 (5)	O1—C2—C8—C9	−177.8 (2)
C5—C6—C7—C7A	0.7 (4)	O2—C8—C9—Cl1	4.7 (4)
C2—O1—C7A—C7	179.5 (3)	C2—C8—C9—Cl1	−175.83 (19)
C2—O1—C7A—C3A	0.2 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9B···O2^{i}	0.97	2.49	3.238 (3)	134

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

Fig. 1