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1-(1-Benzofuran-2-yl)-3-(4-chlorophenyl)prop-2-en-1-one

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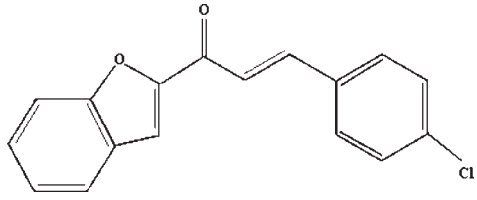
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.115; data-to-parameter ratio = 18.3.

In the title compound, $C_{17}H_{11}ClO_2$, the benzofuran ring system is almost planar (r.m.s. deviation = 0.011 Å) and forms a dihedral angle of 10.53 (6)° with the chlorophenyl ring. No significant intermolecular interactions are observed.

Related literature

For general background to chalcone, see: Dhar (1981). For the biological properties of benzofuran derivatives, see: Nasef *et al.* (1992); Bogolyubsakaya & Perovich (1964); Deshmukh *et al.* (2004); Stanislav *et al.* (2000); Brady *et al.* (1973); Kamal *et al.* (2006); Alejandro *et al.* (2008); Rajesh *et al.* (2006). For related structures, see: Devarajegowda *et al.* (2001); Kant *et al.* (2009).



Experimental

Crystal data

$C_{17}H_{11}ClO_2$
M_r = 282.71
Monoclinic, $P2_1/c$
a = 15.9034 (12) Å
b = 14.1393 (12) Å
c = 5.9572 (5) Å
β = 93.039 (4)°
V = 1337.67 (19) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 K
0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.940, T_{max} = 0.972
12871 measured reflections
3323 independent reflections
2665 reflections with $I > 2\sigma(I)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.02
3323 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5024).

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1-(1-Benzofuran-2-yl)-3-(4-chlorophenyl)prop-2-en-1-one

S. Jeyaseelan, H. C. Devarajegowda, G. Venkatarama, M. Vinduvahini and Alphonsus D'souza

S1. Comment

Chalcones have been recognized as a significant field of study for a long time because of a variety of biological activities as well as they serve as intermediates in the synthesis of a variety of heterocyclic compounds. Several heterocyclic analogues of chalcones have been reported to possess antibacterial, bacteriostatic tuberculostatic, insecticidal, antiparasitic, coronary vasodilating and choleretic activities (Dhar, 1981). Further, benzofuran derivatives have been reported to possess sedative and hypnotic (Nasef *et al.*, 1992), antiinflammatory (Bogolyubsakaya & Perovich, 1964), antidepressant (Deshmukh *et al.*, 2004), analgesic (Stanislav *et al.*, 2000), hypoglycemic (Brady *et al.*, 1973), anticonvulsant (Kamal *et al.*, 2006), antibacterial (Alejandro *et al.*, 2008) and antifungal activities (Rajesh *et al.*, 2006). Owing to these biological activities of benzofuran propenones and in an attempt to study the structure-activity relationship of benzofuran and related systems, it was contemplated to synthesize benzofuryl propenones and the crystal structure of one of them, the title compound, is reported.

The benzofuran ring system is almost planar (r.m.s. deviation 0.011 Å). The dihedral angle between the benzofuran ring system and the chlorophenyl ring is 10.53 (6)°. Bond distances within the aromatic rings are in agreement with those observed in related structures (Devarajegowda *et al.*, 2001; Kant *et al.*, 2009).

S2. Experimental

A mixture of 2-acetylbenzofuran (0.01 mol) and p-chlorobenzaldehyde (0.01 mol) in ethanol (20 ml) was stirred for 24 h in aqueous NaOH (8 ml). It was then diluted with water (100 ml) and acidified with concentrated HCl. The course of the reaction was monitored by TLC using chloroform-carbon disulfide (1:1). The product obtained was filtered, washed with water and recrystallised from ethanol (m.p. 398 K). Spectral data IR (KBr) cm^{-1}: 1650 (C═O), 1620 (C═C stretching in aromatic), 1080 (C-O-C of benzofuran). ^{1}H NMR ($CDCl_3$): 6.67-7.2 (m, 9H, Ar-H), 6.70 (d, 1H, -COCH=), 8.60 (d, 1H, =CH-Ar).

S3. Refinement

H atoms were positioned at calculated positions [C-H = 0.93 Å] and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C).

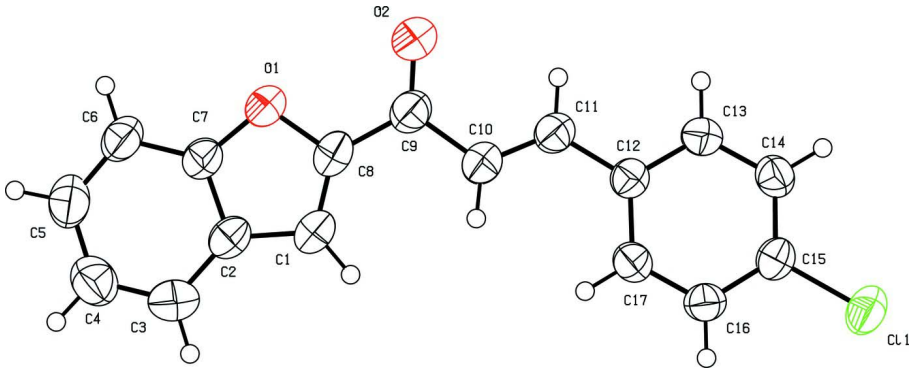

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

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Crystal data

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$c = 5.9572\ (5)$ Å
$\beta = 93.039\ (4)°$
$V = 1337.67\ (19)$ Å^3
$Z = 4$
$F(000) = 584$
$D_x = 1.404$ Mg m^{-3}
Melting point: 398 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3323 reflections
$\theta = 1.3–28.4°$
$\mu = 0.28$ mm^{-1}
$T = 293$ K
Plate, white
0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
$T_{min} = 0.940$, $T_{max} = 0.972$
12871 measured reflections
3323 independent reflections
2665 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.3°$
$h = -21\rightarrow20$
$k = -18\rightarrow18$
$l = -7\rightarrow7$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.115$
$S = 1.02$
3323 reflections
182 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
$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.3221P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.21$ e Å^{-3}
$\Delta\rho_{min} = -0.24$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0117 (16)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.22464 (9)	0.64723 (11)	0.5466 (3)	0.0508 (4)
H1	1.1909	0.6671	0.4232	0.061*
C2	1.31402 (10)	0.64001 (11)	0.5583 (2)	0.0497 (3)
C3	1.37837 (12)	0.65858 (13)	0.4117 (3)	0.0628 (4)
H3	1.3660	0.6820	0.2679	0.075*
C4	1.45972 (12)	0.64125 (15)	0.4865 (3)	0.0717 (5)
H4	1.5031	0.6535	0.3920	0.086*
C5	1.47890 (11)	0.60577 (15)	0.7004 (3)	0.0692 (5)
H5	1.5349	0.5939	0.7447	0.083*
C6	1.41797 (10)	0.58781 (13)	0.8476 (3)	0.0595 (4)
H6	1.4311	0.5644	0.9911	0.071*
C7	1.33559 (9)	0.60625 (11)	0.7727 (2)	0.0485 (3)
C8	1.19823 (9)	0.62016 (11)	0.7456 (3)	0.0517 (4)
C9	1.11355 (10)	0.61170 (12)	0.8310 (3)	0.0540 (4)
C10	1.04368 (10)	0.62421 (13)	0.6625 (3)	0.0560 (4)
H10	1.0546	0.6508	0.5242	0.067*
C11	0.96572 (9)	0.59891 (11)	0.7013 (3)	0.0493 (3)
H11	0.9572	0.5719	0.8407	0.059*
C12	0.89149 (8)	0.60906 (10)	0.5471 (2)	0.0440 (3)
C13	0.81273 (9)	0.58296 (11)	0.6193 (2)	0.0480 (3)
H13	0.8090	0.5549	0.7596	0.058*
C14	0.74015 (9)	0.59803 (11)	0.4862 (3)	0.0501 (3)
H14	0.6879	0.5812	0.5368	0.060*
C15	0.74645 (9)	0.63839 (11)	0.2773 (2)	0.0473 (3)
C16	0.82376 (9)	0.66272 (11)	0.1978 (2)	0.0493 (3)
H16	0.8271	0.6888	0.0553	0.059*
C17	0.89576 (9)	0.64786 (11)	0.3322 (2)	0.0489 (3)
H17	0.9479	0.6638	0.2792	0.059*
O1	1.26490 (6)	0.59456 (8)	0.89122 (17)	0.0552 (3)
O2	1.10294 (8)	0.59470 (11)	1.0286 (2)	0.0755 (4)
Cl1	0.65624 (3)	0.66004 (4)	0.10847 (8)	0.06940 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0515 (8)	0.0488 (8)	0.0506 (8)	0.0031 (6)	−0.0110 (6)	0.0007 (6)

C2	0.0542 (8)	0.0455 (8)	0.0481 (8)	0.0008 (6)	−0.0081 (6)	−0.0025 (6)
C3	0.0775 (11)	0.0621 (10)	0.0489 (8)	0.0026 (8)	0.0042 (8)	0.0027 (7)
C4	0.0633 (11)	0.0824 (13)	0.0706 (11)	−0.0021 (9)	0.0149 (9)	−0.0053 (10)
C5	0.0491 (8)	0.0854 (13)	0.0723 (11)	0.0035 (8)	−0.0041 (8)	−0.0112 (10)
C6	0.0537 (8)	0.0719 (11)	0.0515 (8)	0.0067 (8)	−0.0108 (7)	−0.0022 (8)
C7	0.0486 (7)	0.0495 (8)	0.0466 (7)	−0.0014 (6)	−0.0050 (6)	−0.0008 (6)
C8	0.0480 (7)	0.0488 (8)	0.0567 (8)	0.0013 (6)	−0.0114 (6)	−0.0001 (7)
C9	0.0519 (8)	0.0550 (9)	0.0541 (9)	−0.0010 (7)	−0.0061 (6)	0.0060 (7)
C10	0.0483 (8)	0.0646 (10)	0.0544 (9)	0.0013 (7)	−0.0038 (6)	0.0095 (7)
C11	0.0496 (7)	0.0517 (8)	0.0462 (7)	0.0034 (6)	−0.0015 (6)	0.0019 (6)
C12	0.0445 (7)	0.0425 (7)	0.0450 (7)	0.0025 (6)	0.0014 (5)	−0.0011 (6)
C13	0.0502 (7)	0.0496 (8)	0.0444 (7)	−0.0016 (6)	0.0041 (6)	0.0045 (6)
C14	0.0442 (7)	0.0533 (9)	0.0530 (8)	−0.0057 (6)	0.0052 (6)	0.0002 (7)
C15	0.0456 (7)	0.0467 (8)	0.0490 (7)	−0.0011 (6)	−0.0042 (6)	−0.0034 (6)
C16	0.0529 (8)	0.0536 (8)	0.0414 (7)	−0.0046 (6)	0.0013 (6)	0.0026 (6)
C17	0.0444 (7)	0.0559 (9)	0.0468 (7)	−0.0025 (6)	0.0061 (6)	−0.0008 (6)
O1	0.0499 (6)	0.0655 (7)	0.0491 (6)	0.0006 (5)	−0.0073 (4)	0.0076 (5)
O2	0.0602 (7)	0.1083 (11)	0.0573 (7)	−0.0042 (7)	−0.0050 (5)	0.0175 (7)
Cl1	0.0526 (2)	0.0844 (3)	0.0690 (3)	−0.00645 (19)	−0.01679 (19)	0.0098 (2)

Geometric parameters (Å, º)

C1—C8	1.335 (2)	C9—C10	1.468 (2)
C1—C2	1.423 (2)	C10—C11	1.323 (2)
C1—H1	0.93	C10—H10	0.93
C2—C7	1.389 (2)	C11—C12	1.4641 (19)
C2—C3	1.405 (2)	C11—H11	0.93
C3—C4	1.368 (3)	C12—C13	1.3954 (19)
C3—H3	0.93	C12—C17	1.398 (2)
C4—C5	1.388 (3)	C13—C14	1.382 (2)
C4—H4	0.93	C13—H13	0.93
C5—C6	1.365 (3)	C14—C15	1.377 (2)
C5—H5	0.93	C14—H14	0.93
C6—C7	1.386 (2)	C15—C16	1.384 (2)
C6—H6	0.93	C15—Cl1	1.7352 (15)
C7—O1	1.3690 (18)	C16—C17	1.378 (2)
C8—O1	1.3820 (17)	C16—H16	0.93
C8—C9	1.469 (2)	C17—H17	0.93
C9—O2	1.2216 (19)		
C8—C1—C2	107.24 (13)	C10—C9—C8	115.33 (14)
C8—C1—H1	126.4	C11—C10—C9	122.03 (15)
C2—C1—H1	126.4	C11—C10—H10	119.0
C7—C2—C3	118.89 (14)	C9—C10—H10	119.0
C7—C2—C1	105.49 (14)	C10—C11—C12	126.58 (15)
C3—C2—C1	135.61 (15)	C10—C11—H11	116.7
C4—C3—C2	118.14 (16)	C12—C11—H11	116.7
C4—C3—H3	120.9	C13—C12—C17	118.30 (13)

C2—C3—H3	120.9	C13—C12—C11	119.20 (13)
C3—C4—C5	121.44 (17)	C17—C12—C11	122.45 (13)
C3—C4—H4	119.3	C14—C13—C12	121.23 (13)
C5—C4—H4	119.3	C14—C13—H13	119.4
C6—C5—C4	121.88 (17)	C12—C13—H13	119.4
C6—C5—H5	119.1	C15—C14—C13	118.93 (13)
C4—C5—H5	119.1	C15—C14—H14	120.5
C5—C6—C7	116.70 (16)	C13—C14—H14	120.5
C5—C6—H6	121.7	C14—C15—C16	121.37 (13)
C7—C6—H6	121.7	C14—C15—Cl1	119.95 (12)
O1—C7—C6	126.81 (14)	C16—C15—Cl1	118.68 (11)
O1—C7—C2	110.25 (12)	C17—C16—C15	119.29 (13)
C6—C7—C2	122.94 (15)	C17—C16—H16	120.4
C1—C8—O1	111.44 (14)	C15—C16—H16	120.4
C1—C8—C9	131.92 (14)	C16—C17—C12	120.83 (13)
O1—C8—C9	116.62 (14)	C16—C17—H17	119.6
O2—C9—C10	122.98 (15)	C12—C17—H17	119.6
O2—C9—C8	121.69 (14)	C7—O1—C8	105.57 (12)

C8—C1—C2—C7	0.86 (17)	O2—C9—C10—C11	−14.3 (3)
C8—C1—C2—C3	−178.91 (18)	C8—C9—C10—C11	165.10 (16)
C7—C2—C3—C4	0.8 (2)	C9—C10—C11—C12	179.27 (15)
C1—C2—C3—C4	−179.41 (18)	C10—C11—C12—C13	−176.76 (16)
C2—C3—C4—C5	0.4 (3)	C10—C11—C12—C17	0.4 (3)
C3—C4—C5—C6	−1.0 (3)	C17—C12—C13—C14	−2.4 (2)
C4—C5—C6—C7	0.4 (3)	C11—C12—C13—C14	174.96 (14)
C5—C6—C7—O1	−179.32 (16)	C12—C13—C14—C15	0.9 (2)
C5—C6—C7—C2	0.9 (3)	C13—C14—C15—C16	0.9 (2)
C3—C2—C7—O1	178.67 (14)	C13—C14—C15—Cl1	−178.88 (12)
C1—C2—C7—O1	−1.15 (17)	C14—C15—C16—C17	−1.2 (2)
C3—C2—C7—C6	−1.5 (2)	Cl1—C15—C16—C17	178.57 (12)
C1—C2—C7—C6	178.64 (15)	C15—C16—C17—C12	−0.3 (2)
C2—C1—C8—O1	−0.28 (18)	C13—C12—C17—C16	2.0 (2)
C2—C1—C8—C9	−179.04 (16)	C11—C12—C17—C16	−175.20 (14)
C1—C8—C9—O2	−172.20 (18)	C6—C7—O1—C8	−178.80 (16)
O1—C8—C9—O2	9.1 (2)	C2—C7—O1—C8	0.98 (16)
C1—C8—C9—C10	8.3 (3)	C1—C8—O1—C7	−0.42 (17)
O1—C8—C9—C10	−170.36 (14)	C9—C8—O1—C7	178.55 (13)