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2-(3-Chlorophenyl)chroman-4-one

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Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.083
Data-to-parameter ratio = 14.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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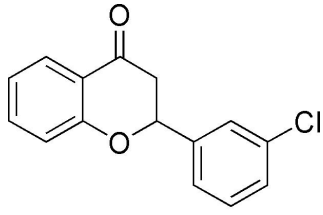
The title compound, $C_{15}H_{11}ClO_2$, was synthesized from 3-(3-chlorophenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one. The pyrone ring adopts a half-chair conformation.

Comment

Flavanones represent important structures of a wide variety of natural products exhibiting various interesting biological activities (Heinisch & Holzer, 1991 Salvatore *et al.*, 1998). It is also found from biological examination that flavanones, such as 2-(2,3-dimethoxyphenyl)chroman-4-one, which we have reported (Wu *et al.*, 2005), has good molluscicidal activity. Thus, the synthesis of flavanones and their derivatives is of great interest in organic chemistry. We report here the crystal structure of the title compound, (I).



(I)

In (I), the pyrone ring adopts a half-chair conformation (Fig. 1). Atom C9 deviates from the plane defined by atoms C6/C8/C9/C1/O1 by 0.679 (3) Å. The dihedral angle between the C8/C9/O1 and C1/C6/C7/C8/O1 planes is 52.13 (14)° and the dihedral angle between the C10–C15 and C1/C6/C7/C8/O1 planes is 78.72 (6)°. The bond lengths, angles and torsion angles in (I) show normal values (Table 1).

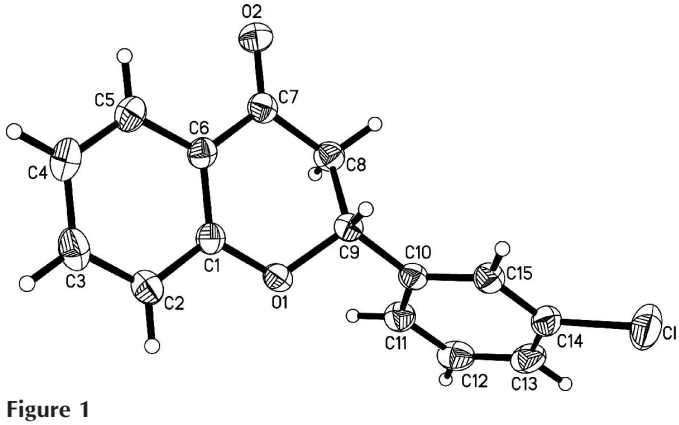


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

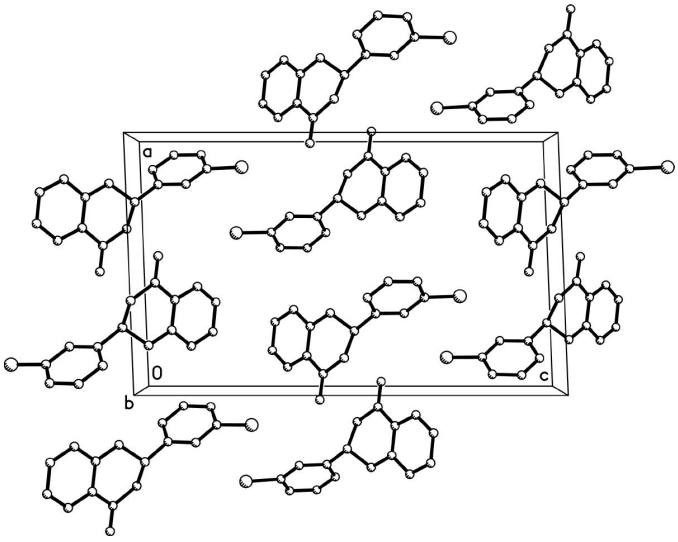


Figure 2
The molecular packing of (I). H atoms have been omitted.

Experimental

The title compound was synthesized from 3-(3-chlorophenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one (4 mmol, 1.03 g) and acetic acid (0.05 g) in ethanol solution (12 ml) at 353 K over a period of 12 h (yield 43%, m.p. 360–362 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a solution in 95% ethanol.

Crystal data

$C_{15}H_{11}ClO_2$
$M_r = 258.69$
Monoclinic, $P2_1/n$
$a = 11.979\ (2)$ Å
$b = 5.202\ (1)$ Å
$c = 19.773\ (3)$ Å
$\beta = 92.22\ (2)^\circ$
$V = 1231.1\ (4)$ Å^3
$Z = 4$
$D_x = 1.396$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 30 reflections
$\theta = 3.4$–12.4°
$\mu = 0.30$ mm^{-1}
$T = 292\ (2)$ K
Block, colourless
0.52 × 0.42 × 0.42 mm

Data collection

Siemens P4 diffractometer
ω scans
Absorption correction: multi-scan (*SHELXTL*; Sheldrick, 1997)
$T_{min} = 0.853$, $T_{max} = 0.882$
2790 measured reflections
2296 independent reflections
1314 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.5^\circ$
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 6$
$l = -23 \rightarrow 23$
3 standard reflections
every 97 reflections
intensity decay: 1.8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.083$
$S = 0.87$
2296 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0361P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0140 (14)

Table 1
Selected geometric parameters (Å, °).

Cl—C14	1.745 (2)	C6—C7	1.470 (3)
O1—C1	1.366 (2)	C7—C8	1.505 (3)
O1—C9	1.450 (2)	C8—C9	1.508 (2)
C1—C6	1.402 (2)		
C1—O1—C9	113.58 (14)	C1—C6—C7	119.90 (18)
O1—C1—C2	117.26 (18)	C6—C7—C8	114.88 (17)
O1—C1—C6	122.39 (18)	C7—C8—C9	111.08 (17)
C9—O1—C1—C2	−154.59 (17)	C1—C6—C7—O2	175.19 (19)
C9—O1—C1—C6	24.0 (3)	C1—C6—C7—C8	−3.3 (3)
O1—C1—C2—C3	176.57 (18)	C6—C7—C8—C9	−28.6 (2)
C6—C1—C2—C3	−2.1 (3)	C1—O1—C9—C8	−56.2 (2)
O1—C1—C6—C5	−175.45 (17)	C7—C8—C9—C10	179.61 (17)
O1—C1—C6—C7	6.9 (3)	Cl—C14—C15—C10	−177.41 (15)

All H atoms were placed in calculated positions and treated using a riding model, with C—H distances of 0.93–0.98 Å and U_{iso}(H) values of $1.2U_{eq}$(C).

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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