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**Key indicators**

Single-crystal X-ray study  
 T = 294 K  
 Mean  $\sigma(C-C)$  = 0.002 Å  
 R factor = 0.042  
 wR factor = 0.125  
 Data-to-parameter ratio = 16.8

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

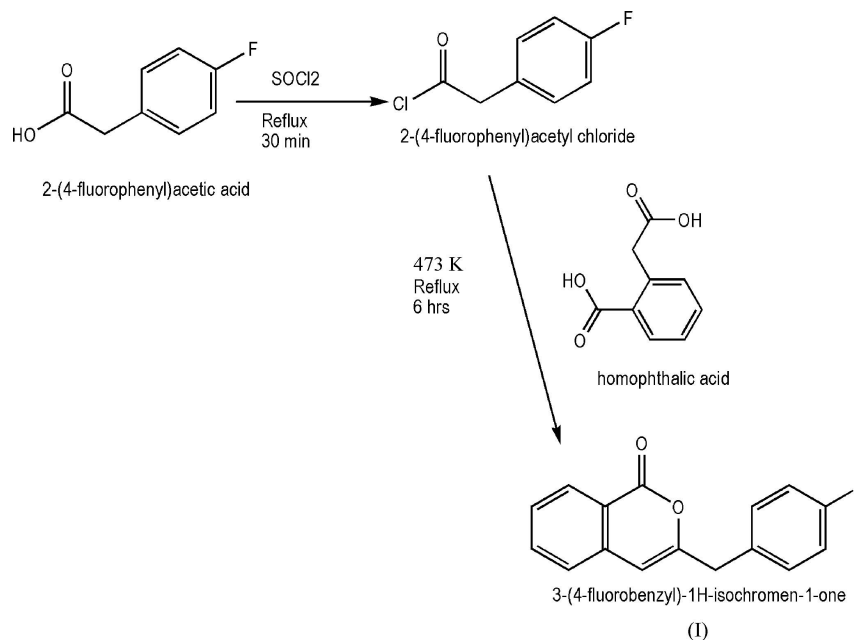
## 3-(4-Fluorobenzyl)isocoumarin

In the title compound, C<sub>16</sub>H<sub>11</sub>FO<sub>2</sub>, a synthetic isocoumarin, the benzene ring is not perpendicular to the planar isocoumarin ring system, the dihedral angle being 75.32 (3)°. Intermolecular C—H···O hydrogen bonds may be effective in the stabilization of the crystal structure.

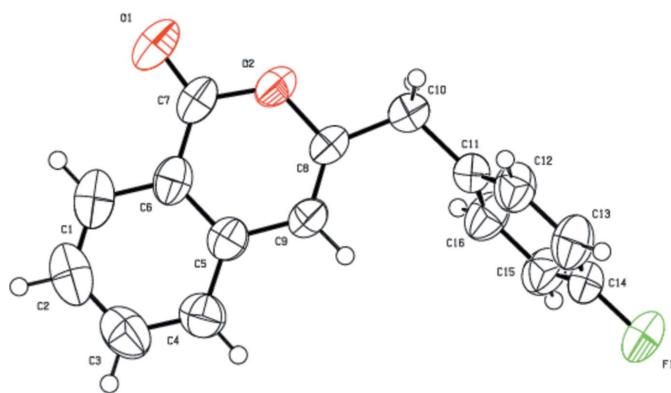
Received 8 November 2006  
 Accepted 10 November 2006

### Comment

The isocoumarin nucleus is an abundant structural motif in natural products (Barry, 1964). Many constituents of the steadily growing class of known isocoumarins exhibit valuable biological properties such as antifungal (Sturtz *et al.*, 2002), antitumor or cytotoxic, anti-inflammatory, anti-allergic (Rossi *et al.*, 2003) and enzyme inhibitory activity (Powers *et al.*, 2002). Naturally occurring haloisocoumarins and halogeno-3,4-dihydroisocoumarins are very rare; however, a few examples of naturally occurring chlorine-containing isocoumarins are known (Thomas & Jens, 1999). In view of the importance of this class of compounds, the title compound, (I), has been synthesized and its crystal structure is reported here.



In (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The isocoumarin ring system is planar, with a maximum displacement from the mean plane of 0.0379 (7) Å° for C8. The benzene ring is not perpendicular to the isocoumarin ring, the dihedral angle being 75.32 (3)°.



**Figure 1**  
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

In the crystal structure, intermolecular C—H...O hydrogen bonds (Table 1) may be effective in the stabilization of the crystal structure. Dipole–dipole and van der Waals interactions are also effective in the molecular packing.

## Experimental

A mixture of 4-fluorophenylacetic acid (7.5 g, 48.7 mmol) and thionyl chloride (4.5 ml, 37.8 mmol) was heated for 30 min in the presence of a few drops of DMF under reflux at 343 K to give 4-fluorophenylacetyl chloride. Completion of the reaction was indicated by the cessation of gas evolution. Removal of excess thionyl chloride was carried out under reduced pressure to afford 4-fluorophenylacetyl chloride. Homophthalic acid (2.0 g, 11 mmol) was then added and the solution was refluxed for 6 h at 473 K with stirring. The reaction mixture was extracted with ethyl acetate (3 × 100 ml); an aqueous solution of sodium carbonate (5%, 200 ml) was added to remove the unreacted homophthalic acid. The organic layer was separated, concentrated and chromatographed on silica gel using petroleum ether (313–353 K fractions) as eluent to afford the title compound (yield 78%; m.p. 454 K). Colorless single crystals suitable for X-ray crystallographic analysis were obtained by slow evaporation of an ethyl acetate solution.

### Crystal data

$C_{16}H_{11}FO_2$	$Z = 4$
$M_r = 254.25$	$D_x = 1.353 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 16.3696 (16) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$b = 5.5359 (5) \text{ \AA}$	$T = 294 (2) \text{ K}$
$c = 14.1406 (14) \text{ \AA}$	Block, colorless
$\beta = 103.011 (2)^\circ$	$0.28 \times 0.22 \times 0.20 \text{ mm}$
$V = 1248.5 (2) \text{ \AA}^3$	

### Data collection

Bruker SMART CCD area-detector diffractometer	6998 measured reflections
$\omega$ and $\varphi$ scan	2883 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	1969 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.972$ , $T_{\max} = 0.981$	$R_{\text{int}} = 0.020$
	$\theta_{\max} = 28.3^\circ$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.1403P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.125$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.01$	$\Delta\rho_{\max} = 0.11 \text{ e \AA}^{-3}$
2883 reflections	$\Delta\rho_{\min} = -0.18 \text{ e \AA}^{-3}$
172 parameters	
H-atom parameters constrained	

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C9-H9A\cdots O1^i$	0.93	2.47	3.3157 (17)	151

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

H atoms were positioned geometrically, with C—H = 0.93 and 0.97  $\text{\AA}$  for aromatic and methylene H, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1999); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

The authors gratefully acknowledge funds from the URF project, Quaid-I-Azam University, Islamabad, Pakistan.

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