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## Key indicators

Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.007$  Å  
 $R$  factor = 0.035  
 $wR$  factor = 0.106  
Data-to-parameter ratio = 14.2

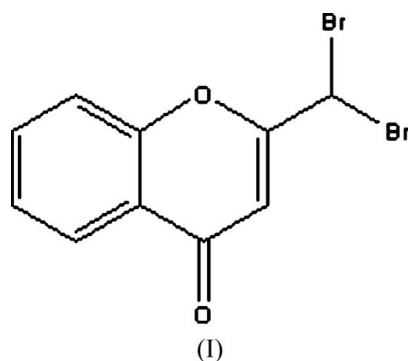
For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

2-(Dibromomethyl)-4*H*-chromen-4-one

In the crystal structure of the title compound,  $\text{C}_{10}\text{H}_6\text{Br}_2\text{O}_2$ , centrosymmetric hydrogen-bonded dimers are formed *via*  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds.  $\pi-\pi$  stacking interactions involving these dimers are also observed.

## Comment

Chromones are one of the most important groups of biological compounds in nature, and are used as a synthetic lead for drug discovery. Recently, the structural modification of the chromone scaffold, with the introduction of heterocyclic substituents at either the 2- or 3-position, has attracted considerable attention. Some chromones bearing a heterocyclic thioether group have been reported to be anticancer agents (Khim *et al.*, 2004). The title compound, (I), is an important intermediate for the synthesis of chromone derivatives.



The molecular structure of (I) is illustrated in Fig. 1. Atom C8, with attached atom H8, forms a hydrogen bond to atom O2 of a symmetry-related molecule. This leads to the formation of hydrogen-bonded dimers, as shown in Fig. 2 (details are given in Table 1). As a result, a ten-membered ring is formed whose topological motif corresponds to the first level graph-set descriptor  $R_2^2(10)$  (Bernstein *et al.*, 1995). Weak  $\pi-\pi$  stacking is observed, with the distance between the benzene ring centroids,  $\text{Cg}1\cdots\text{Cg}1b$ , being 3.672 (3) Å (see Fig. 2 for details). These interactions are very similar to those observed in our previous report on the crystal structure of 3-(4,6-dimethylpyrimidin-2-yl)-2-methylchromen-4-one (Huang *et al.*, 2005).

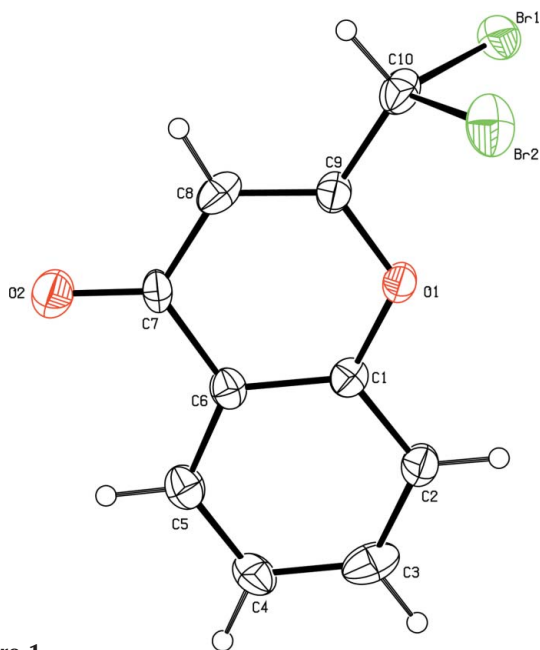
## Experimental

Compound (I) was synthesized according to the literature procedure of Khim *et al.* (2004). Crystals suitable for X-ray analysis were grown from acetone at 277 K.

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**Figure 1**

A view of the molecular structure of (I), showing the atom-labelling scheme and with displacement ellipsoids drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

**Crystal data**

$C_{10}H_6Br_2O_2$   
 $M_r = 317.97$   
 Monoclinic,  $P2_1/c$   
 $a = 8.2343$  (14) Å  
 $b = 10.3445$  (18) Å  
 $c = 12.047$  (2) Å  
 $\beta = 96.884$  (3)°  
 $V = 1018.7$  (3) Å<sup>3</sup>  
 $Z = 4$

$D_x = 2.073$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 2048 reflections  
 $\theta = 2.6$ – $25.1$ °  
 $\mu = 7.93$  mm<sup>-1</sup>  
 $T = 292$  (2) K  
 Block, pink  
 $0.30 \times 0.20 \times 0.10$  mm

**Data collection**

Bruker SMART 4K CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.179$ ,  $T_{\max} = 0.453$   
 5018 measured reflections

1802 independent reflections  
 1496 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$   
 $\theta_{\text{max}} = 25.1$ °  
 $h = -9 \rightarrow 9$   
 $k = -11 \rightarrow 12$   
 $l = -12 \rightarrow 14$

**Refinement**

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.106$   
 $S = 1.13$   
 1802 reflections  
 127 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0485P)^2 + 1.7251P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.008$   
 $\Delta\rho_{\text{max}} = 0.56$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.47$  e Å<sup>-3</sup>

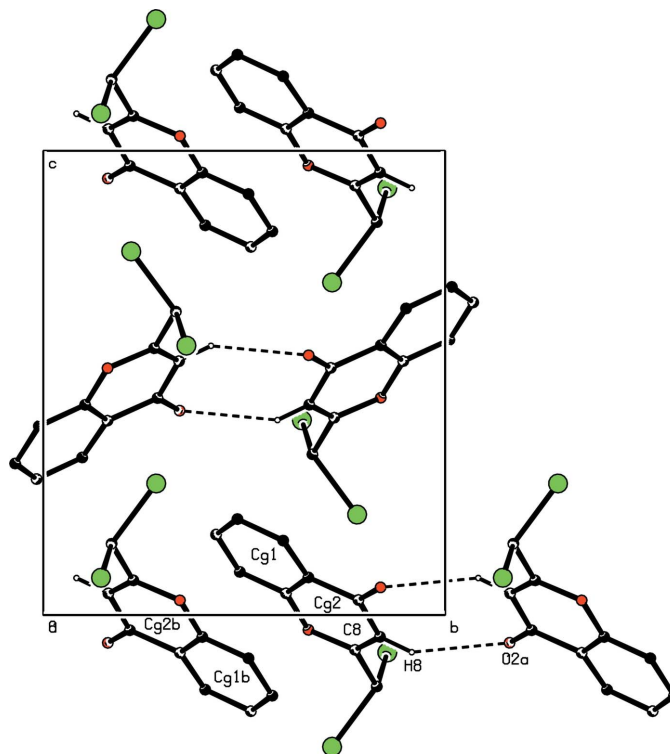
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C8-H8\cdots O2^i$	0.93	2.54	3.342 (6)	145

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

H atoms were placed in calculated positions and treated as riding atoms, with C–H bond distances in the range 0.93–0.98 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

**Figure 2**

A view of the crystal packing in compound (I), showing the formation of the hydrogen-bonded dimers and the  $\pi$ – $\pi$  stacking. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted. [Symmetry codes: (a)  $-x + 1, -y + 2, -z$ ; (b)  $1 - x, 1 - y, -z$ .]

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2001); software used to prepare material for publication: SHELXTL.

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**References**

- Bernstein, J., Davis, R. E., Shimon, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.  
 Bruker (1997). SMART. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (1999). SAINT. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Bruker (2001). SHELXTL. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Huang, W., Teng, D., Zhou, Z. & Yang G. (2005). *Acta Cryst.* **E61**, o2510–o2512.  
 Khim, Y.-W., Hackett, J. C. & Brueggemeier, R. W. (2004). *J. Med. Chem.* **47**, 4032–4040.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.