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## Key indicators

Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.054  
 $wR$  factor = 0.151  
Data-to-parameter ratio = 16.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

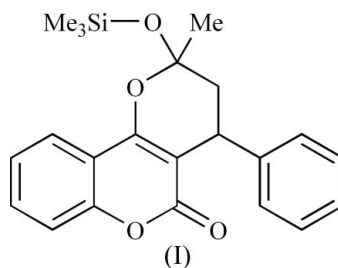
## 2-Methyl-4-phenyl-2-(trimethylsilyloxy)-3,4-dihydro-2H,5H-pyrano[3,2-c][1]-benzopyran-5-one

In the title compound,  $\text{C}_{22}\text{H}_{24}\text{O}_4\text{Si}$ , the coumarin system is essentially planar and the pyran ring adopts a half-chair conformation. There are intermolecular  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\pi$  interactions in the crystal structure.

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## Comment

The cycloaddition chemistry of *o*-quinone methides has attracted considerable interest (Nair *et al.*, 2001). In our recent research work on the cycloaddition reactions of *o*-quinone methides derived from 4-hydroxycoumarin, we have prepared the title compound, (I), which is obtained from the cycloaddition reaction between coumarin quinone methide and an excess amount of trimethyl[(1-methylethenyl)oxy]silane. As part of this study, we have undertaken the X-ray crystallographic analysis of (I) in order to elucidate the conformation of this cycloadduct product.

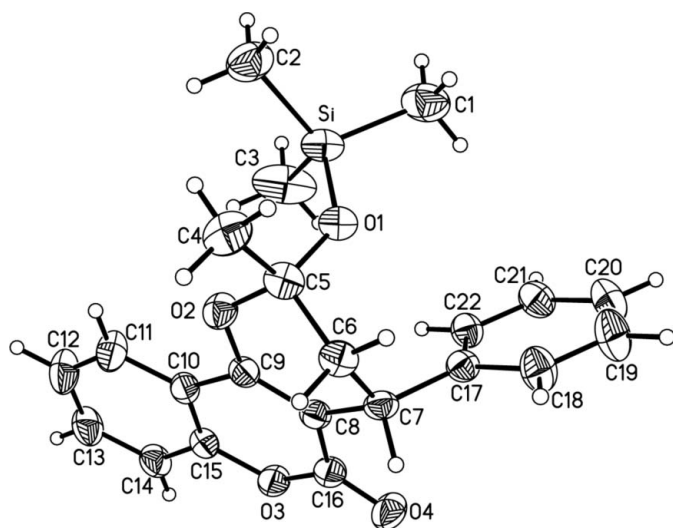


The bond lengths and angles in (I) (Fig. 1 and Table 1) are in good agreement with those found in the related compound 2-methyl-2-(trimethylsilyloxy)-3,4-dihydro-2H,5H-pyrano[3,2-c][1]benzopyran-5-one (Peng *et al.*, 2005). The coumarin system is essentially planar. The dihedral angle between the coumarin unit and the benzene ring ( $\text{C}17-\text{C}22$ ) is  $73.8(3)^\circ$ . The pyran ring ( $\text{C}5-\text{C}9/\text{O}2$ ) adopts a half-chair conformation, with atoms  $\text{C}5$  and  $\text{C}6$  deviating from the  $\text{C}7-\text{C}9/\text{O}2$  plane by  $0.232(4)$  and  $-0.466(4)$  Å, respectively.

In the crystal structure, the molecular packing is stabilized by intermolecular  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\pi$  interactions (Table 2) involving the aromatic rings.

## Experimental

Under argon, a mixture of 4-hydroxycoumarin, 3 equivalents of trimethyl[(1-methylethenyl)oxy]silane and an excess amount of benzaldehyde were suspended in dry dioxane and refluxed for about 20 h. Compound (I) was isolated by column chromatography of the reaction mixture on silica gel after evaporation of the solvent, in 27% yield. Single crystals of (I) were obtained by slow evaporation of a petroleum ether–ethyl acetate (2:1 *v/v*) solution.



**Figure 1**  
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

#### Crystal data

$C_{22}H_{24}O_4Si$	$Z = 4$
$M_r = 380.50$	$D_x = 1.227 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 10.038 (2) \text{ \AA}$	$\mu = 0.14 \text{ mm}^{-1}$
$b = 12.396 (3) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 16.853 (3) \text{ \AA}$	Block, colourless
$\beta = 100.74 (3)^\circ$	$0.40 \times 0.31 \times 0.28 \text{ mm}$
$V = 2060.3 (8) \text{ \AA}^3$	

#### Data collection

Enraf–Nonius CAD-4 diffractometer	4029 independent reflections
$\omega/2\theta$ scans	2297 reflections with $I > 2\sigma(I)$
Absorption correction: $\psi$ scan (XCAD4; Harms & Wocadlo, 1995)	$R_{\text{int}} = 0.117$
$T_{\text{min}} = 0.931$ , $T_{\text{max}} = 0.962$	$\theta_{\text{max}} = 26.0^\circ$
4268 measured reflections	3 standard reflections every 200 reflections
	intensity decay: none

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.05P)^2 + P]$
$R[F^2 > 2\sigma(F^2)] = 0.054$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.151$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
4029 reflections	$\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
245 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.0157 (13)

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Si—O1	1.651 (2)	O4—C16	1.206 (3)
O1—C5	1.396 (3)	C5—C6	1.506 (4)
C5—O1—Si	135.16 (19)	C15—O3—C16	121.4 (2)
C9—O2—C5	117.4 (2)	C5—C6—C7	112.9 (2)

**Table 2**

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1B $\cdots$ O3 <sup>i</sup>	0.96	2.58	3.482 (4)	156
C14—H14 $\cdots$ O4 <sup>ii</sup>	0.93	2.55	3.463 (4)	168
C6—H6A $\cdots$ Cg(B) <sup>iii</sup>	0.97	2.81	3.773 (3)	175
C21—H21 $\cdots$ Cg(A) <sup>iv</sup>	0.93	2.96	3.815 (4)	153

Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x + 2, -y + 1, -z$ ; (iii)  $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ ; (iv)  $-x + 1, -y + 1, -z$ . Notes: Cg(A) and Cg(B) denote the centroids of the aromatic rings C10–C15 and C17–C22, respectively

The H atoms were included in the riding-model approximation, with C—H distances of 0.93, 0.96, 0.97 and 0.98  $\text{\AA}$  for aromatic, methyl, methylene and methine H atoms, respectively, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{aromatic, methylene and methine C})$  or  $1.5U_{\text{eq}}(\text{methyl C})$ .

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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