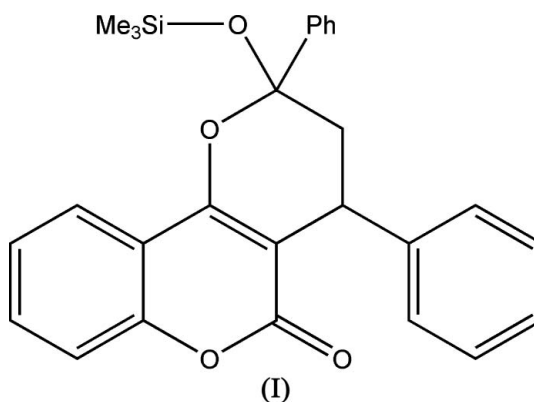


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Republic of ChinaCorrespondence e-mail:  
shenyongmiao@nju.org.cn**Key indicators**Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.047  
 $wR$  factor = 0.139  
Data-to-parameter ratio = 14.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**2,4-Diphenyl-2-(trimethylsilyloxy)-3-dihydro-  
2H,5H-pyrano[3,2-c][1]benzopyran-5-one**In the title compound,  $\text{C}_{27}\text{H}_{26}\text{O}_4\text{Si}$ , the coumarin ring system  
is essentially planar and the pyran ring adopts a half-chair  
conformation.Received 6 March 2006  
Accepted 10 March 2006**Comment**The recognition of the synthetic potential of heterocyclic  
quinone methides has aroused considerable interest in their  
generation and subsequent transformations. (Nair *et al.*, 2001).  
We have recently investigated the cycloaddition reaction  
between coumarin quinone methide, 3-phenylmethylene-2H-  
1-benzopyran-2,4(3H)-dione and trimethyl[(1-phenylethen-  
yl)oxy]silane, which gave the title compound, (I), as one of the  
products. An X-ray crystallographic analysis was undertaken  
to establish its structure and conformation.

In the title structure (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and are in good agreement with the related compound 2-methyl-2-(trimethylsilyloxy)-3,4-dihydro-2H,5H-pyrano[3,2-c][1]benzopyran-5-one (Peng *et al.*, 2005). No classical intermolecular hydrogen bonds were found in the crystal structure but there is an intramolecular  $\text{C}-\text{H}\cdots\text{O}$  hydrogen-bonding interaction (Table 2). The dihedral angle between the heterocyclic plane (C19–C21/O4/C22/C27) and the fused benzene ring is  $4.74^\circ$ . The pyran ring (C7–C9/C19/C20/O2) adopts a half-chair conformation, with atom C7 deviating from the C9/C19/C20/O2 plane by  $0.596\text{ \AA}$ .

**Experimental**

The title compound, (I), was prepared by the reaction of 4-hydroxycoumarin, 3 equivalents of trimethyl[(1-phenylethenyl)oxy]silane and an excess of benzaldehyde. The mixture in dry dioxane was refluxed for about 18 h. Compound (I) was isolated by column chromatography of the reaction mixture on silica gel after evapora-

tion of the solvent, in 31% yield. Single crystals of (I) were obtained by slow evaporation of a petroleum ether–ethyl acetate (3:1 v/v) solution.

Crystal data

$C_{27}H_{26}O_4Si$   
 $M_r = 442.57$   
 Monoclinic,  $P2_1/n$   
 $a = 12.223 (2) \text{ \AA}$   
 $b = 12.740 (3) \text{ \AA}$   
 $c = 15.113 (3) \text{ \AA}$   
 $\beta = 91.59 (3)^\circ$   
 $V = 2352.5 (8) \text{ \AA}^3$   
 $Z = 4$

$D_x = 1.250 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 25 reflections  
 $\theta = 10\text{--}13^\circ$   
 $\mu = 0.13 \text{ mm}^{-1}$   
 $T = 298 (2) \text{ K}$   
 Block, colorless  
 $0.30 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Enraf–Nonius CAD-4 diffractometer  
 $\omega/2\theta$  scans  
 Absorption correction:  $\psi$  scan (XCAD4; Harms & Wocadlo, 1995)  
 $T_{\min} = 0.962$ ,  $T_{\max} = 0.973$   
 4333 measured reflections  
 4129 independent reflections

2773 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$   
 $\theta_{\text{max}} = 25.0^\circ$   
 $h = 0 \rightarrow 14$   
 $k = 0 \rightarrow 15$   
 $l = -17 \rightarrow 17$   
 3 standard reflections every 200 reflections  
 intensity decay: none

Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.139$   
 $S = 1.00$   
 4129 reflections  
 290 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.08P)^2 + 0.0023P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.007$   
 $\Delta\rho_{\text{max}} = 0.26 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$   
 Extinction correction: SHELXL97  
 Extinction coefficient: 0.0219 (18)

Table 1

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

Si–O1	1.6648 (16)	Si–C10	1.846 (3)
O1–Si–C10	101.86 (11)	C19–O2–C9	119.15 (16)
C9–O1–Si	131.77 (14)	C9–C8–C7	113.06 (17)
C4–C5–C7–C20	–2.4 (3)	C7–C8–C9–O2	–55.1 (2)

Table 2

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

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
C14–H14A $\cdots$ O2	0.93	2.38	2.708 (3)	100

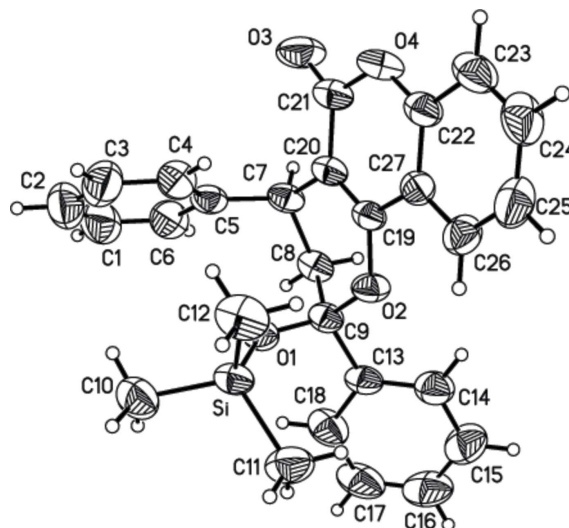


Figure 1

The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

The H atoms were positioned geometrically and were refined as riding, with C–H = 0.93–0.98  $\text{\AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  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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