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## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.047  
 $wR$  factor = 0.137  
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-(4-*tert*-Butylbenzyl)-3-phenylinden-1-one

The title compound,  $\text{C}_{26}\text{H}_{24}\text{O}$ , was obtained from the reaction of 2-[(4-*tert*-butyl)phenylmethyl]-1,3-diphenylpropane-1,3-dione with acetic anhydride. The reaction yielded 92% of the product. The crystal structure confirms the formation of the five-membered ring from the parent dione.

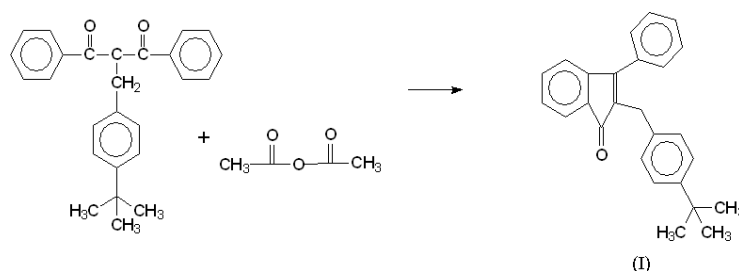
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## Comment

The title compound, (I), was synthesized in order to explore the stability of various indenone ozonides; 2-methyl-3-phenylinden-1-one has been shown to form stable ozonides (Karban *et al.*, 1978). It was also synthesized in order to assess the effect of a *tert*-butyl group on the stability of an ozonide derived from a substituted 2-methyl-3-phenylinden-1-one. Other substituents, such as methyl, bromo, and nitro, were also tested. The preparation of the indenones followed methods described by Guidrinence *et al.* (1963) in which 2-[(4-*tert*-butyl)phenylmethyl]-1,3-diphenylpropane-1,3-dione undergoes dehydration with ring closure to form the indenone. Compound (I), the *tert*-butyl derivative, gave a 92% yield and produced an ozonide that was stable for several days.



The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are presented in Table 1. The crystal structure reveals an indenone nucleus with a phenyl substituent in the 3-position and a 4-*tert*-butylbenzyl substituent in the 2-position. The O1—C1 bond has a length which represents a double bond. For the five-membered ring of the indenone, the bond assignment is confirmed in that C2—C3 is an acceptable double bond and the other non-aromatic bonds are of appropriate lengths for single bonds. The 3-phenyl ring (C10—C15) is tilted  $54.94$  ( $5$ )° from the indenone plane.

## Experimental

Benzyl-1,3-diphenylpropane-1,3-dione (10.8 mmol) was dissolved in dry 1,2-dichloroethane (65 ml). A mixture of concentrated sulfuric acid (10 ml) and acetic anhydride (50 ml), both ice cold, was added slowly. The mixture was stirred for 24 h at room temperature. Ice-cold water (250 ml) was added and stirring continued, allowing the

mixture to be extracted with diethyl ether. The organic layer of ether/dichloroethane was dried with anhydrous magnesium sulfate and the solvent was then evaporated, leaving a crystalline product. The product formed yellow rhombic crystals with a melting point of 422–423 K. The  $^1\text{H}$  NMR spectrum showed peaks at  $\delta$  1.27 (s, 9H),  $\delta$  3.65 (s, 2H) and  $\delta$  7.35 (m, 13H). The IR spectrum showed a peak at  $1705\text{ cm}^{-1}$  (C=O).

#### Crystal data

$\text{C}_{26}\text{H}_{24}\text{O}$   
 $M_r = 352.45$   
 Monoclinic,  $P2_1/c$   
 $a = 10.0255$  (3) Å  
 $b = 10.1273$  (4) Å  
 $c = 19.4485$  (6) Å  
 $\beta = 91.931$  (2)°  
 $V = 1973.51$  (12) Å<sup>3</sup>  
 $Z = 4$

$D_x = 1.186\text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 Cell parameters from 5432 reflections  
 $\theta = 2.3\text{--}23.9^\circ$   
 $\mu = 0.07\text{ mm}^{-1}$   
 $T = 298$  (2) K  
 Block, yellow  
 $0.17 \times 0.09 \times 0.08\text{ mm}$

#### Data collection

Bruker X8 APEX CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.988$ ,  $T_{\max} = 0.994$   
 22 372 measured reflections

4039 independent reflections  
 2905 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.031$   
 $\theta_{\text{max}} = 26.4^\circ$   
 $h = -12 \rightarrow 12$   
 $k = -12 \rightarrow 12$   
 $l = -23 \rightarrow 24$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.137$   
 $S = 1.05$   
 4039 reflections  
 247 parameters  
 H-atom parameters constrained

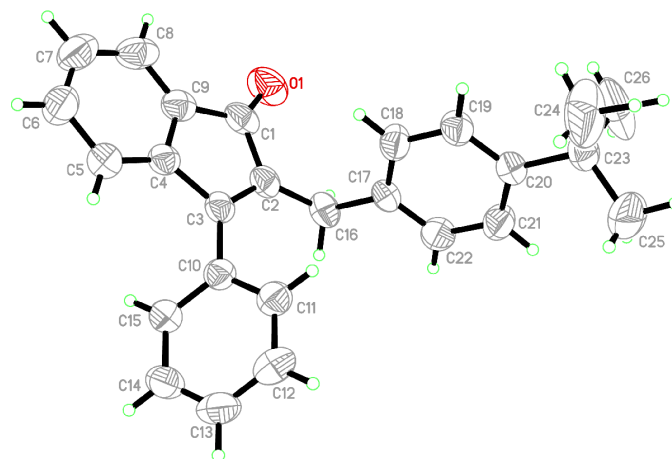
$w = 1/[\sigma^2(F_o^2) + (0.0687P)^2 + 0.3278P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.16\text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.22\text{ e \AA}^{-3}$

**Table 1**

Selected bond lengths (Å).

O1—C1	1.219 (2)	C2—C3	1.351 (2)
C1—C9	1.491 (3)	C3—C4	1.497 (2)
C1—C2	1.494 (2)		

H atoms were placed in calculated positions (C—H = 0.93 Å) and H-atom isotropic displacement parameters were fixed and refined as riding, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .



**Figure 1**

The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level

Data collection: *APEX2* (Bruker, 2003); cell refinement: *APEX2*; data reduction: *SAINT-Plus* (Bruker, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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