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## Key indicators

Single-crystal X-ray study  
 $T = 298$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.044  
 $wR$  factor = 0.119  
Data-to-parameter ratio = 16.7For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 1-Chloro-4-octyloxy-10-thiaanthracen-9-one

In the title compound,  $\text{C}_{21}\text{H}_{23}\text{ClO}_2\text{S}$ , the three fused rings are roughly coplanar. The two benzene rings are twisted by a dihedral angle of  $7.15$  ( $15$ )°.Received 4 April 2006  
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## Comment

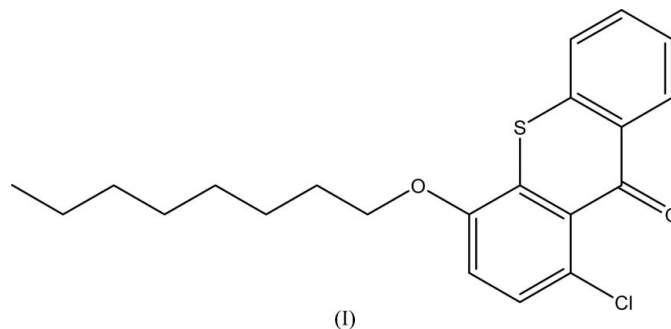
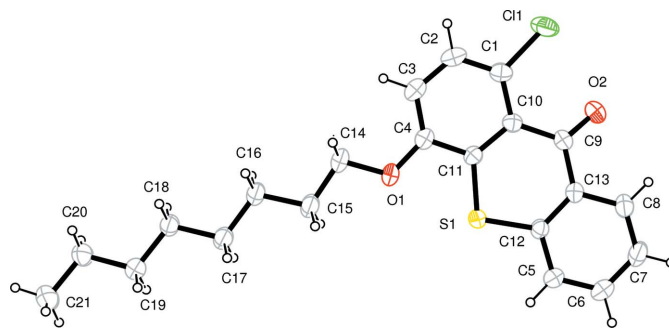
Thioxanthone derivatives are good photoinitiators with excellent capabilities in UV-curing materials. They have been widely used in UV-curing applications because they absorb at a longer UV wavelength and have a faster photocuring speed than other photoinitiators (Allen *et al.*, 1994, 1999). In a continuation of our research on new synthetic pathways of the title compound, (I) (Liu *et al.*, 2003), we have obtained pale-yellow crystals from ethanol suitable for X-ray structural analysis.The molecular structure of (I) is illustrated in Fig. 1. The three fused rings are roughly coplanar, the largest deviation being  $0.171$  ( $2$ ) Å for C9. However, the two benzene rings are slightly twisted, making a dihedral angle of  $7.15$  ( $15$ )°. The aliphatic carbon chain is also roughly planar and is nearly

Figure 1

The molecular structure of compound (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radii.

coplanar with the thioxanthone system, making a dihedral angle of only 7.73 (14)°.

Weak C—H···O hydrogen bonds result in the formation of a dimer arranged around an inversion centre (Fig. 2).

### Experimental

The title compound was prepared from 1-chloro-4-hydroxythioxanthone and 1-bromooctane, according to the procedure of Liu *et al.* (2003). A solution of the compound in ethanol was concentrated gradually at room temperature to afford pale-yellow prisms.

#### Crystal data

C <sub>21</sub> H <sub>25</sub> ClO <sub>2</sub> S	$V = 956.01 (18) \text{ \AA}^3$
$M_r = 374.91$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.302 \text{ Mg m}^{-3}$
$a = 10.0899 (11) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.2174 (11) \text{ \AA}$	$\mu = 0.32 \text{ mm}^{-1}$
$c = 10.5201 (11) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 114.223 (1)^\circ$	Prism, pale yellow
$\beta = 94.019 (1)^\circ$	$0.40 \times 0.20 \times 0.15 \text{ mm}$
$\gamma = 101.309 (1)^\circ$	

#### Data collection

Enraf–Nonius CAD-4 diffractometer	3798 independent reflections
$\omega$ scans	2989 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.012$
$T_{\text{min}} = 0.883$ , $T_{\text{max}} = 0.954$	$\theta_{\text{max}} = 26.3^\circ$
5761 measured reflections	3 standard reflections
	frequency: 60 min
	intensity decay: 2.1%

#### Refinement

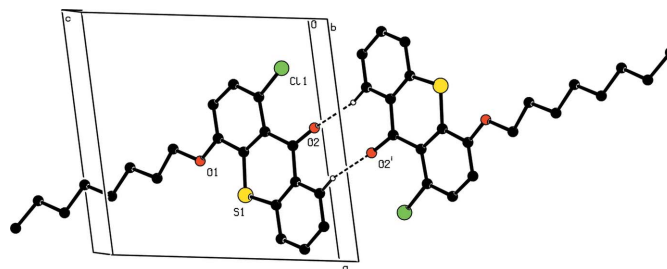
Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.2576P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.119$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.41 \text{ e \AA}^{-3}$
3798 reflections	$\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$
227 parameters	
H-atom parameters constrained	

**Table 1**

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$C8-H8\cdots O2^i$	0.93	2.46	3.360 (3)	163

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



**Figure 2**

A view showing the formation of a dimer through C—H···O hydrogen bonds (dashed lines). H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry code: (i)  $-x + 1, -y + 2, -z$ .]

H atoms were positioned geometrically and treated as riding on their parent C atoms, with C—H distances of 0.93 (C<sub>aromatic</sub>), 0.96 (CH<sub>3</sub>) and 0.97 Å (CH<sub>2</sub>), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ , or  $1.5U_{\text{eq}}(\text{C})$  for methyl groups.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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