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1-Chloro-4-propoxythioxanthone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.042
wR factor = 0.128
Data-to-parameter ratio = 13.1

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

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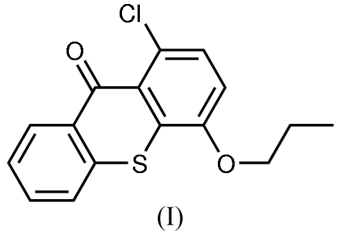
In the title compound (systematic name: 1-chloro-4-propoxy-10-thiaanthracen-9-one), $C_{16}H_{13}ClO_2S$, the asymmetric unit contains two parallel molecules. In both molecules, the three rings in the thioxanthone moiety are coplanar, the deviations being within the range ±0.086 (3) Å.

Comment

Thioxanthone derivatives are good photoinitiators with excellent capabilities in UV-curing materials. The title compound was first explored by Arthur *et al.* (1992). It was widely used in UV-curing fields because it had a longer UV absorbing wavelength and a more rapid photocuring speed (Norman *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 yellow crystals from ethanol suitable for X-ray structural analysis.



(I)

The two essentially identical molecules forming the asymmetric unit of (I) are shown in Fig. 1. The two independent molecules are roughly parallel to each other, with a head-to-head arrangement. In both molecules, the three rings in the thioxanthone moiety are coplanar, the deviations being within the range ±0.086 (3) Å.

Experimental

The title compound was prepared from 1-chloro-4-hydroxythioxanthone and 1-bromo-propane, according to the procedure of Liu *et al.* (2003).

Crystal data

$C_{16}H_{13}ClO_2S$
M_r = 304.78
Triclinic, $P\overline{1}$
a = 11.298 (3) Å
b = 11.841 (2) Å
c = 12.776 (3) Å
α = 108.28 (2)°
β = 112.84 (2)°
γ = 98.71 (2)°
V = 1420.9 (7) Å^3
Z = 4
D_x = 1.425 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 11.7–13.3°
μ = 0.41 mm^{-1}
T = 293 K
Prism, yellow
0.35 × 0.25 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.017$
$\omega/2\theta$ scans	$\theta_{max} = 25.2^\circ$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -1 \rightarrow 13$
$T_{min} = 0.878$, $T_{max} = 0.934$	$k = -14 \rightarrow 14$
5950 measured reflections	$l = -15 \rightarrow 14$
5106 independent reflections	3 standard reflections
3225 reflections with $I > 2\sigma(I)$	every 60 min
	intensity decay: 0.3%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.769P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.042$	$(\Delta/\sigma)_{max} = 0.016$
$wR(F^2) = 0.128$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
$S = 1.01$	$\Delta\rho_{min} = -0.48$ e Å^{-3}
5106 reflections	
391 parameters	
H-atom parameters constrained	

H atoms were positioned geometrically and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2 (or 1.5 for methyl H atoms) times the equivalent isotropic displacement parameters of their parent atoms, and C—H distances were set equal to 0.93 Å for H atoms bonded to phenyl rings, 0.96 Å for methyl H atoms and 0.97 Å for the remainder. One of the propyl groups displays large displacement ellipsoids with unrealistic C—C bond lengths. This propyl group could be modeled as disordered, with occupancy factors in the ratio 0.66:0.34.

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

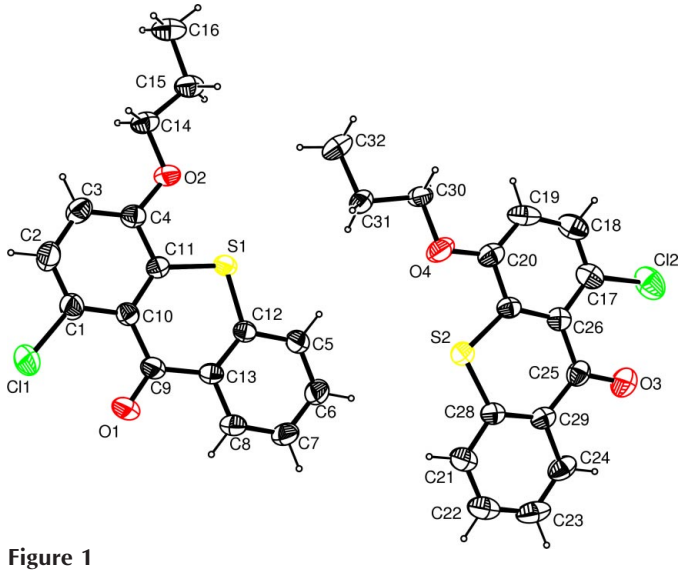


Figure 1
The structure of the asymmetric unit of (I), with 30% probability displacement ellipsoids.

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