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Diisopropyl (1,3-dithiolan-2-ylidene)malonate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.010 Å
R factor = 0.090
wR factor = 0.205
Data-to-parameter ratio = 14.0

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

The title compound, $C_{12}H_{18}O_4S_2$, exhibits fungicidal activity. A short S···S intermolecular contact [3.576 (3)Å] is observed in the crystal structure, which is further stabilized by C—H···O intermolecular interactions, forming molecular chains along the *b* axis.

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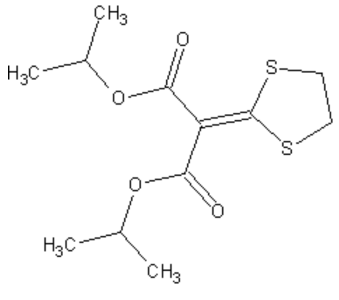
Comment

An important aspect in the rational design of bioactive molecules involves relating chemical structure to biological activity (Lewis *et al.*, 1991). The conformation of the molecule is found to influence the levels of biological activity. Correlation of the results obtained from X-ray crystallography with biological activity has aided in the chemical design of a few active agrochemicals. The activity of a series of triazolyl ketone herbicides (Anderson *et al.*, 1983) has been investigated, along with the fungicidal activities of *N*-phenylsuccinamides (Zenei *et al.*, 1988). There have been relatively few reports of attempts to correlate structure with biological activity. In view of this, the structure determination of other agrochemicals exhibiting fungicidal activity becomes important, so that the conformation in the solid state is known and the nature of binding features with the active site of the enzyme becomes more meaningful.



(I)

The molecular structure of the title compound, (I), is depicted in Fig. 1. The bond lengths S2—C3 and S1—C2 are 1.747 (5) and 1.803 (6) Å, respectively, indicating differences in the electronic environments of the S atoms. Atoms C1 and C2 of the 1,3-dithiolane ring deviate by −0.336 (6) and 0.356 (6) Å, respectively, from the least-squares plane, indicating a half-chair (or twist) conformation. C—H···O intermolecular interactions link the molecules, forming molecular chains which are related by a *b* glide plane $(-x+\frac{3}{2}, y+\frac{1}{2}, z)$ (Fig. 2). In addition, a short S···S intermolecular contact [3.576 (3) Å] is observed in the crystal structure.

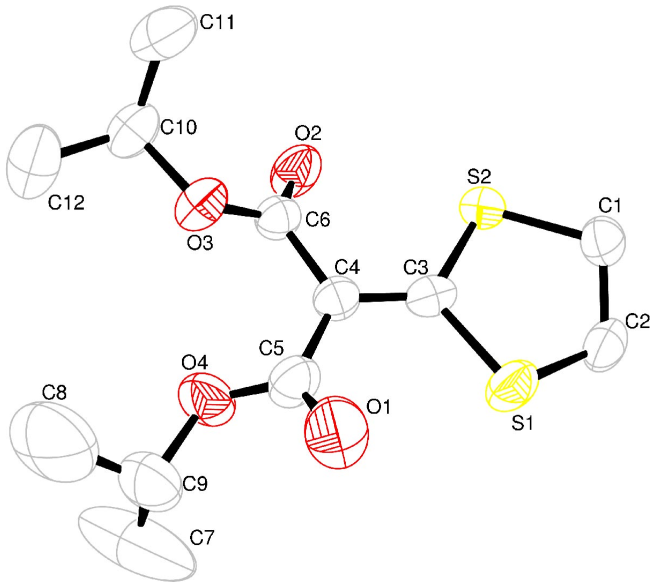


Figure 1
The molecular structure of (I), showing 40% probability ellipsoids. H atoms have been omitted.

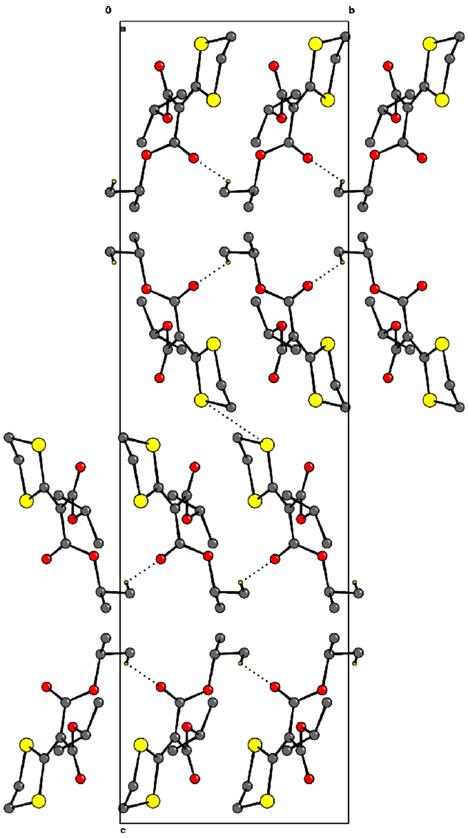


Figure 2
Packing diagram of (I), showing the S···S short contact and C—H···O intermolecular interactions as dashed lines. Other H atoms have been omitted.

Experimental

The title compound was obtained from Rallis India, Bangalore. Single crystals were grown by slow evaporation of a methanol/hexane mixture at 278 K.

Crystal data

$C_{12}H_{18}O_4S_2$
$M_r = 290.40$
Orthorhombic, *Pbca*
$a = 10.400\ (7)$ Å
$b = 9.117\ (6)$ Å
$c = 32.09\ (2)$ Å
$V = 3043\ (3)$ Å^3
$Z = 8$
$D_x = 1.268$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 675 reflections
$\theta = 1.9$–$24.4°$
$\mu = 0.35$ mm^{-1}
$T = 293\ (2)$ K
Block, colourless
0.23 × 0.11 × 0.02 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.943$, $T_{\max} = 0.993$
20 345 measured reflections
2681 independent reflections
1925 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.057$
$\theta_{\max} = 25.0°$
$h = -12 \rightarrow 11$
$k = -10 \rightarrow 10$
$l = -38 \rightarrow 34$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.090$
$wR(F^2) = 0.205$
$S = 1.22$
2681 reflections
191 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0874P)^2 + 1.215P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.31$ e Å^{-3}
$\Delta\rho_{\min} = -0.22$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—C2	1.494 (8)	C4—C5	1.466 (7)
S1—C2	1.803 (6)	C6—C4	1.477 (6)
S1—C3	1.756 (4)	O2—C6	1.199 (5)
S2—C1	1.811 (5)	O3—C6	1.330 (5)
S2—C3	1.747 (5)	C5—O1	1.196 (6)
C3—C4	1.364 (6)	O4—C5	1.315 (6)
C3—S1—C2	96.0 (2)	C3—C4—C5	119.7 (4)
C3—S2—C1	96.4 (3)	C3—C4—C6	119.2 (4)
C4—C3—S1	123.0 (4)	C5—C4—C6	121.0 (4)
C4—C3—S2	123.5 (3)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7*C*···O1$^{\rm i}$	0.96	2.51	3.281 (19)	138

Symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} + y, z$.

The methyl H atoms were constrained to an ideal geometry, with C—H = 0.96 Å and $U_{\rm iso}({\rm H}) = 1.5U_{\rm eq}({\rm C})$, but were allowed to rotate freely about the C—C bond. The remaining H atoms were located in a difference Fourier map and refined isotropically. Because of their greater rotational freedom, the isopropyl groups exhibit some positional disorder with greater vibrational motion, particularly of atoms C7 and C8. This leads to unusually high values of their displacement parameters.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SIR*92 (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et*

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al., 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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