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(*Z*)-2-Methylsulfanyl-1,4-di-*p*-tolylbut-2-ene-1,4-dione

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.005 Å
R factor = 0.068
wR factor = 0.152
Data-to-parameter ratio = 15.8

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

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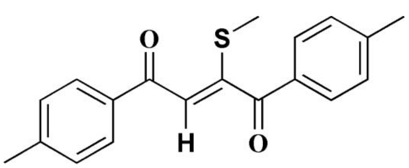
The title compound, $C_{19}H_{18}O_2S$, displays a *trans* configuration with respect to the central C═C double bond. The dihedral angle between the two aromatic rings is 67.91 (5)°.

Comment

1,4-Dicarbonyl compounds are widely used as synthetic building blocks for further elaboration into substituted cyclopentenones, such as jasmones, rethorolones, cuparenones and prostaglandins, and five-membered heterocyclic compounds, such as furans, pyrroles, thiophenes and pyridazines (Ellison, 1973; Yuguchi *et al.*, 2004). As a part of our ongoing investigation into 1,4-dicarbonyl compounds (Chen *et al.*, 2007), we present here the structure of the title compound, (I) (Fig. 1).



(I)

The dihedral angle between the two aromatic rings is 67.91 (5)°. The structure is stabilized by intermolecular C—H···O hydrogen bonds (Table 1).

Experimental

Compound (I) was prepared according to the method described by Yin *et al.* (2006). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane–methanol (1:1, *v*/*v*) solution at 283 K.

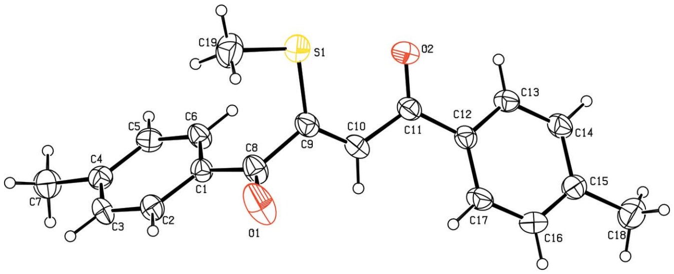


Figure 1
The molecular structure of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented by circles of arbitrary size.

Crystal data

$C_{19}H_{18}O_2S$
$M_r = 310.39$
Orthorhombic, $P2_12_12_1$
$a = 5.7812$ (6) Å
$b = 7.5573$ (8) Å
$c = 37.412$ (4) Å
$V = 1634.5$ (3) Å^3
$Z = 4$
$D_x = 1.261$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.20$ mm^{-1}
$T = 297$ (2) K
Block, yellow
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
12645 measured reflections
3199 independent reflections
2450 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.052$
$\theta_{\rm max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.152$
$S = 1.09$
3199 reflections
202 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0684P)^2 + 0.2905P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.017$
$\Delta\rho_{\rm max} = 0.28$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.16$ e Å^{-3}
Absolute structure: Flack (1983), 1287 Friedel pairs
Flack parameter: 0.07 (16)

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C16—H16$\cdots$O2$^{\rm i}$	0.93	2.43	3.318 (5)	159

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

All H atoms were refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic H, and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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