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(*Z*)-1,4-Bis(4-methoxyphenyl)-2-(methylsulfanyl)but-2-ene-1,4-dione

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Key indicators

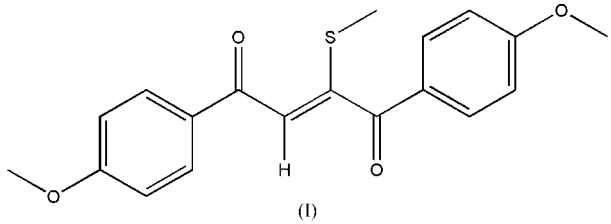
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.050
wR factor = 0.129
Data-to-parameter ratio = 16.8

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

The title compound, $C_{19}H_{18}O_4S$, displays a *trans* configuration with respect to the central C=C double bond. The dihedral angle between the two aromatic rings is 81.67 (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). We report here the structure of the title compound, (I) (Fig. 1).



(I)

The molecule contains two planar fragments, O1/O2/C1–C8 and S1/O3/O4/C9–C18, which are almost perpendicular to each other, forming a dihedral angle of 84.22 (4)°.

The crystal packing is stabilized by a weak π–π interaction between the C2–C7 benzene rings at (*x*, *y*, *z*) and (2 − *x*, 1 − *y*, 1 − *z*), with their centroids separated by 3.6997 (12) Å.

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 CH_2Cl_2–CH_3OH (1:1, *v*/*v*) solution at 283 K.

Crystal data

$C_{19}H_{18}O_4S$
M_r = 342.39
Monoclinic, $P2_1/n$
a = 5.6728 (6) Å
b = 17.9498 (18) Å
c = 16.6998 (16) Å
β = 92.225 (2)°
V = 1699.2 (3) Å^3
Z = 4
D_x = 1.338 Mg m^{-3}
Mo *Kα* radiation
μ = 0.21 mm^{-1}
T = 298 (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: none
9848 measured reflections
3694 independent reflections
2975 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 27.0°

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Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0606P)^2 + 0.3174P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.050$	$(\Delta/\sigma)_{max} = 0.005$
$wR(F^2) = 0.129$	$\Delta\rho_{max} = 0.25$ e Å^{-3}
$S = 1.06$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
3694 reflections	
220 parameters	
H-atom parameters constrained	

All H atoms were refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C) for aromatic H, and C—H = 0.96 Å and U_{iso}(H) = 1.5U_{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: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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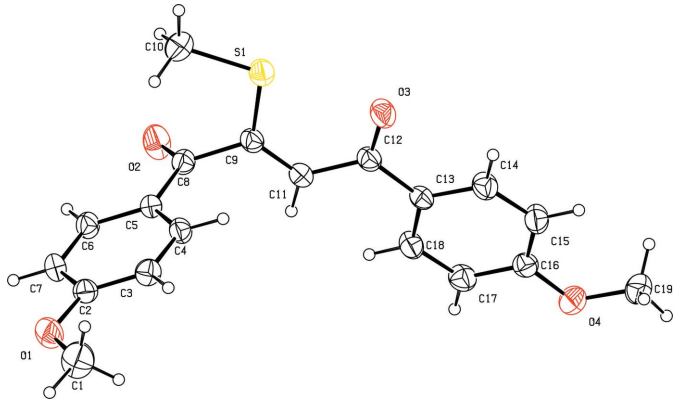

Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

References

Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1999). *SAINT*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.

Ellison, R. (1973). *Synthesis*, pp. 397–412.

Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

Yin, G., Zhou, B., Meng, X., Wu, A. & Pan, Y. (2006). *Org. Lett.* **8**, 2245–2248.

Yuguchi, M., Tokuda, M. & Orito, K. (2004). *J. Org. Chem.* **69**, 908–914.