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1-(4-Methoxyphenyl)-3,3-bis(methylsulfanyl)-2-phenylprop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.172
Data-to-parameter ratio = 22.5

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

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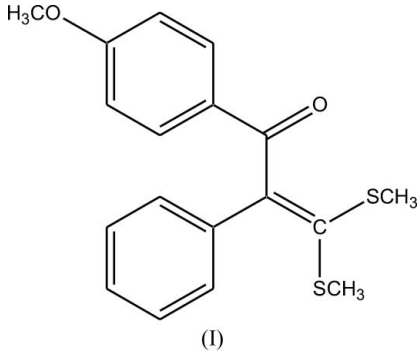
In the title compound, $C_{18}H_{18}O_2S_2$, there are two independent and conformationally similar molecules in the asymmetric unit. In one of the molecules, the dihedral angle between the two aromatic rings is 77.1 (2)°, and in the other it is 78.2 (2)°. The two independent molecules are linked by a C—H···π interaction.

Comment

Chalcone and its derivatives are natural and synthetic compounds belonging to the flavonoid family. They possess a broad spectrum of biological activities, including antibacterial, antihelmintic, amoebicidal, anti-ulcer, antiviral, insecticidal, antiprotzoal, anticancer, cytotoxic and immunosuppressive activities (Dimmock *et al.*, 1999). Chalcone derivatives were also reported to inhibit the destruction of the myelin sheath in the central nervous system of multiple sclerosis patients and were thus useful in controlling the progressive nature of the disease (Edwards *et al.*, 1989). Chalcone derivatives are notable for their excellent blue light transmittance and good crystallizability (Fichou *et al.*, 1988; Kitaoka *et al.*, 1990; Zhao *et al.*, 2000). Sulfur-containing compounds act as simple diuretics (Crawford and Kennedy, 1959). Against this background, the crystal structure of the title compound, (I), has been determined and the results are presented here.



(I)

The asymmetric unit of (I) contains two independent and conformationally similar molecules, *A* and *B* (Fig. 1). Bond lengths and angles of these two molecules agree with each other, and the C—S distances agree well with those observed in a similar structure (Woźniak *et al.*, 2006). The dihedral angle between the two aromatic rings is 77.1 (2)° in molecule *A* and 78.2 (2)° in *B*. In both molecules the methoxy group is almost coplanar with the attached ring.

A weak C—H···S intramolecular interaction is observed in both *A* and *B*. The two independent molecules are linked *via* a

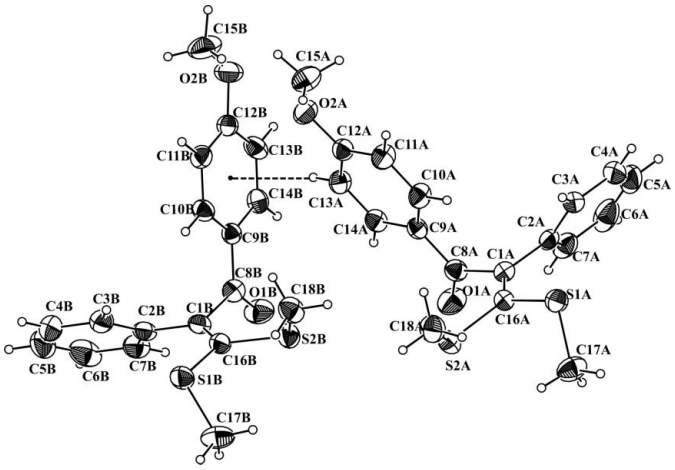


Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids. The dashed line indicates a C—H···π interaction.

C—H···π interaction involving the C9*B*–C14*B* benzene ring (Table 1).

Experimental

Benzyl *p*-anisyl ketone (5.0 mmol) in dry THF (20 ml) and carbon disulfide (5.1 mmol) in dry THF (10 ml) were added slowly to a stirred suspension of 50% NaH (0.24 g, 10 mmol) in dry THF (4 ml) under a nitrogen atmosphere at 273 K. The reaction mixture was stirred at 273–278 K for 10 min. Methyl iodide (13.0 mmol) in dry THF (10 ml) was then added and the reaction mixture was stirred at 273–278 K for 2 h. The solution was then treated with saturated aqueous ammonium chloride solution (50 ml) and the layers were separated. The aqueous layer was extracted with chloroform (4 × 15 ml), and the combined organic layers were dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give an oil. This was crystallized from chloroform and hexane (3:7) to give a yellow crystalline solid (yield 82%).

Crystal data

$C_{18}H_{18}O_2S_2$
M_r = 330.44
Monoclinic, $P2_1/a$
a = 16.471 (3) Å
b = 9.879 (4) Å
c = 22.065 (8) Å
β = 109.362 (17)°
V = 3387.2 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 293 (2) K
0.24 × 0.22 × 0.19 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
9240 measured reflections
8931 independent reflections
4621 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
3 standard reflections
frequency: 60 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.172
S = 1.02
8931 reflections
397 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

*Cg*1 is the centroid of the C9*B*–C14*B* benzene ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3*A*—H3*A*···S1*A*	0.93	2.85	3.218 (4)	105
C3*B*—H3*B*···S1*B*	0.93	2.82	3.212 (4)	106
C13*A*—H13*A*···*Cg*1	0.93	2.78	3.701 (3)	171

H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93 or 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

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: *ZORTEP* (Zsolnai, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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