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## Key indicators

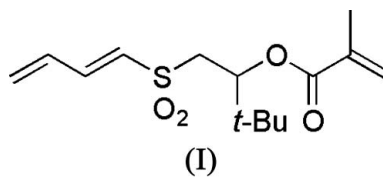
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.035  
 $wR$  factor = 0.097  
Data-to-parameter ratio = 22.4For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.1-[(*E*)-Butadienylsulfonyl]-3,3-dimethylbut-2-yl  
methacrylate

The title compound,  $\text{C}_{14}\text{H}_{22}\text{O}_4\text{S}$ , was synthesized as a precursor for intramolecular Diels–Alder cycloaddition reactions. The (*E*)-buta-1,3-dienyl and methacrylate ester systems adopt an *s-trans* conformation in the solid state, with the two  $\pi$  units in both cases being almost coplanar.

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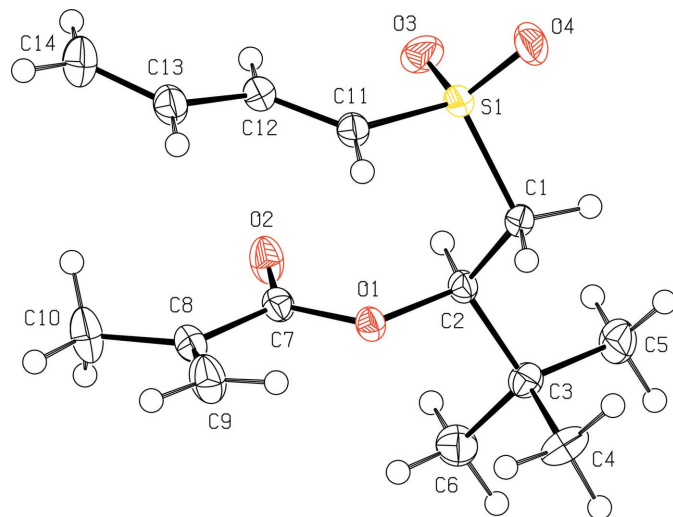
## Comment

The title compound, (I), was prepared as part of a study of the potential utility of sulfone-based tethers in intramolecular Diels–Alder cycloaddition reactions (Chumachenko *et al.*, 2005). Its structure in the solid state has been established at 100 K by single-crystal X-ray diffraction.



The molecule consists of the two essentially planar buta-1,3-dienyl and methacrylate  $\pi$  systems, connected by a flexible tether consisting of atoms C1 and C2 and the  $\text{SO}_2$  group. Similar to all other structurally characterized compounds with a buta-1,3-dienyl substituent listed in the Cambridge Structural Database (CSD, Version 5.27 plus January 2006 update; Allen 2002; 24 compounds), the buta-1,3-dienyl group exhibits the sterically more favoured *s-trans* conformation. Due to the lack of repulsive interactions involving the alkene H atoms, the conformations of methacrylate ester groups found in the CSD are approximately evenly distributed between *s-trans* and *gauche* (42 *s-trans*, 33 *gauche*). In compound (I), the  $\text{C}=\text{O}$  and  $\text{C}=\text{C}$   $\pi$  bonds of the methacrylate moiety are disposed in the *s-trans* conformation. The methacrylate ester  $\text{C}-\text{O}$  bond adopts the intrinsically more stable *Z* conformation (Elieil & Wilen, 1994), which is further stabilized in (I) through minimized steric interactions involving the *tert*-butyl group. The r.m.s. deviation from planarity for the methacrylate  $\pi$  system is 0.0255  $\text{\AA}$ , while that for the *s-trans* buta-1,3-dienyl group is 0.0661  $\text{\AA}$ .

The two unsaturated units are folded back on each other at the flexible tether, thus giving the whole molecule an overall U shape in the solid state (Fig. 1). The methacrylate and butadienyl groups are in close spatial proximity, bringing atoms O1 and C11, C7 and C12, and C8 and C13 into close contact with each other. For these atoms, a modest  $\pi$ – $\pi$  interaction can be assumed. A more perfect stacking of the two  $\pi$  systems is prevented by the *s-trans* conformation of the butadienyl



**Figure 1**  
The molecular structure of (I), showing 50% probability displacement ellipsoids.

group, which brings the terminal  $=\text{CH}_2$  group close in space to the methyl group of the methacrylate group, thus prising the two  $\pi$  systems apart. The spacing between the two unsaturated groups at the tether, represented by the distance  $\text{O1}\cdots\text{C11}$ , is 3.056 (1) Å, while that at the remote end, expressed by the distance  $\text{C8}\cdots\text{C13}$ , is 3.705 (2) Å. The intermediate distance  $\text{C7}\cdots\text{C12}$  is 2.383 (2) Å, and the angle between the planes of the two  $\pi$  systems is 19.52 (8)°.

A weak  $\text{S}=\text{O}\cdots\text{H}-\text{C}$  intermolecular interaction is observed, which seems to contribute to the packing pattern observed for (I). Atom O4 of the  $\text{SO}_2$  group is in close contact with the atom H1A of a neighbouring molecule. The distances  $\text{O4}\cdots\text{H1A}^i$  and  $\text{O4}\cdots\text{C1}^i$  are 2.351 and 3.296 (1) Å, respectively [symmetry code: (i)  $1 - x, -y, 2 - z$ ]. Two such  $\text{S}=\text{O}\cdots\text{H}-\text{C}$  interactions result in the association of two molecules of (I) to form a dimer in the solid state. No effect of this interaction is observed on the  $\text{S}=\text{O}$  bond distance, which is basically identical to the  $\text{S1}-\text{O3}$  distance [1.439 (1) and 1.4425 (9) Å, respectively].

## Experimental

The title compound, (I), was synthesized as described by Chumachenko *et al.* (2005). Single crystals were grown as large colourless blocks from a toluene solution by slow cooling to 278 K.

### Crystal data

$\text{C}_{14}\text{H}_{22}\text{O}_4\text{S}$	$D_x = 1.199 \text{ Mg m}^{-3}$
$M_r = 286.38$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5932 reflections
$a = 8.8062$ (5) Å	$\theta = 2.3\text{--}30.4^\circ$
$b = 16.888$ (1) Å	$\mu = 0.21 \text{ mm}^{-1}$
$c = 10.6858$ (6) Å	$T = 298$ (2) K
$\beta = 93.102$ (1)°	Block, colourless
$V = 1586.9$ (2) Å <sup>3</sup>	$0.60 \times 0.40 \times 0.40 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	3945 independent reflections
$\omega$ scans	3607 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS in SAINTE-Plus; Bruker, 2003)	$R_{\text{int}} = 0.021$
$T_{\text{min}} = 0.873, T_{\text{max}} = 0.919$	$\theta_{\text{max}} = 28.3^\circ$
16205 measured reflections	$h = -11 \rightarrow 11$
	$k = -22 \rightarrow 22$
	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0536P)^2 + 0.4386P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.097$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.45 \text{ e \AA}^{-3}$
3945 reflections	$\Delta\rho_{\text{min}} = -0.24 \text{ e \AA}^{-3}$
176 parameters	
H-atom parameters constrained	

**Table 1**

Selected bond lengths (Å).

$\text{C7}-\text{O2}$	1.2060 (13)	$\text{C11}-\text{S1}$	1.7480 (11)
$\text{C7}-\text{O1}$	1.3433 (12)	$\text{C12}-\text{C13}$	1.4524 (15)
$\text{C7}-\text{C8}$	1.4922 (14)	$\text{C13}-\text{C14}$	1.3264 (18)
$\text{C8}-\text{C9}$	1.3346 (16)	$\text{O3}-\text{S1}$	1.4392 (10)
$\text{C8}-\text{C10}$	1.4849 (16)	$\text{O4}-\text{S1}$	1.4425 (9)
$\text{C11}-\text{C12}$	1.3313 (15)		

All H atoms were positioned geometrically, with C—H distances in the range 0.95–1.0 Å. They were treated as riding, with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H or  $1.2U_{\text{eq}}(\text{C})$  for all others. Methyl H atoms were allowed to rotate to best fit the experimental data. The s.u. values of the cell parameters are taken from the software, recognizing that the values are unreasonably small (Herbstein, 2000).

Data collection: SMART (Bruker, 2002); cell refinement: SAINTE-Plus (Bruker, 2003); data reduction: SAINTE-Plus; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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