

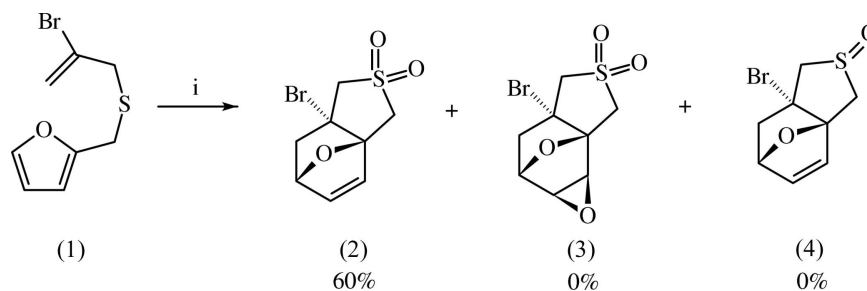
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## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.035  
 $wR$  factor = 0.069  
Data-to-parameter ratio = 14.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.5-Bromo-10-oxa-3-thiatricyclo[5.2.1.0<sup>1,5</sup>]-  
dec-8-ene 3,3-dioxideIn the title compound,  $\text{C}_8\text{H}_9\text{BrO}_3\text{S}$ , the six-membered ring has a boat conformation, the two O-containing five-membered rings have envelope conformations and the tetrahydrothiophene ring has a twist conformation. The molecules are linked only by weak van der Waals interactions.Received 2 August 2006  
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## Comment

Sulfones are a core functional group in both organic and medicinal chemistry because of their versatile synthetic utility and their use as inhibitors of various types of enzymatic processes (Supuran *et al.*, 2003). Alkenyl sulfones are well known for their ability to inhibit many types of cysteine proteases (Roush *et al.*, 1998; Palmer *et al.*, 1995). Alkenyl sulfones are reversible inhibitors of these enzymes through conjugated addition of the thiol of the active-site cysteine residue. In the synthetic sense, alkenyl sulfones have come to play an important role, acting as efficient Michael acceptors and as  $\pi$  donors in cycloaddition reactions (Simpkins, 1990). We have been studying the intramolecular Diels–Alder reaction of furan-cored compounds in which the tether connecting the diene and dienophile consists of three atoms and contains a heteroatom (Demircan & Parsons, 2002; Büyükgüngör *et al.*, 2005). The title compound, (2), can be derived simply from bromofuranylthioether, (1) (see scheme).The Br–C bond distance, 1.961 (3) Å, is not significantly different from the value reported for a pure Br–C single bond (1.94 Å; Toprak *et al.*, 2001). The six-membered ring is in a boat conformation. The two O-containing five-membered rings adopt envelope conformations, whereas the tetrahydrothiophene ring adopts a twist conformation. The molecules are linked only by weak van der Waals interactions.

## Experimental

To a solution of *meta*-chloroperbenzoic acid (*m*-CPBA) (300 mg, 1.2 mmol), which had previously been purified and recrystallized from dry diethyl ether, in dichloromethane (10 ml), cooled to 273 K,

was added dropwise a solution of 2-(2-bromoallylsulfanyl)methylfuran (0.6 mmol) in dichloromethane (10 ml) over a period of 3 min. The reaction mixture was stirred at room temperature for 4 h and then diluted with cold 4% sodium bicarbonate solution (4 ml). The organic layer was separated, washed with water (20 ml) and concentrated *in vacuo*. The crude residue was heated in toluene (10 ml) for a further 24 h at 383 K. The solvent was then removed under reduced pressure and the resulting solid was subjected to flash column chromatography to afford (2).

#### Crystal data

$C_8H_9BrO_3S$	$Z = 8$
$M_r = 265.12$	$D_x = 1.899 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 10.1723 (6) \text{ \AA}$	$\mu = 4.63 \text{ mm}^{-1}$
$b = 10.3446 (9) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 17.6278 (10) \text{ \AA}$	Plate, colorless
$V = 1854.9 (2) \text{ \AA}^3$	$0.50 \times 0.27 \times 0.03 \text{ mm}$

#### Data collection

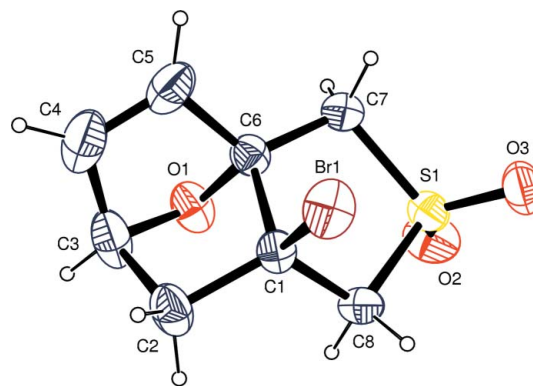
Stoe IPDS-2 diffractometer	12215 measured reflections
$\omega$ scans	1823 independent reflections
Absorption correction: integration ( <i>X-RED32</i> ; Stoe & Cie, 2002)	1370 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.232$ , $T_{\max} = 0.870$	$R_{\text{int}} = 0.102$
	$\theta_{\text{max}} = 26.0^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.024P)^2 + 1.8112P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.069$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.95$	$\Delta\rho_{\text{max}} = 0.30 \text{ e \AA}^{-3}$
1823 reflections	$\Delta\rho_{\text{min}} = -0.34 \text{ e \AA}^{-3}$
130 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Atoms H3, H4 and H5, attached to C3, C4 and C5, respectively, were refined freely [ $C-H = 0.91 (6)$ – $0.98 (5) \text{ \AA}$ ]. The other H atoms were refined using a riding model, with  $C-H = 0.97 \text{ \AA}$  and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).



**Figure 1**

The molecular structure of the title compound, with the atom-numbering scheme and 50% probability displacement ellipsoids.

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