The title compound, C_{11}H_{11}BrO_{3}S, was prepared by reaction of sodium allylsulfinate with \( p \)-bromophenacyl bromide to confirm the identity of the former.

**Comment**

Thermal desulfination of allylic sulfinic acids is a synthetically useful procedure for the regio- and stereospecific synthesis of alkenes. In general, allylic sulfinic acids are unstable, with spontaneous retro-ene desulfination occurring readily at room temperatures with allylic transposition of the double bond (Braverman, 1990).

In our studies on the preparation of allyl sulfinic acid (4) by acid cleavage of the corresponding tributyltin allylic sulfinate, (3), the unstable acid was isolated as the sodium salt, (2), by immediate quenching with sodium bicarbonate (Hiscock et al., 1995). The products obtained in this reaction did not, however, give satisfactory combustion analysis and, to confirm its identity, it was derivatized with \( p \)-bromophenacyl bromide. Spectroscopic analysis (\(^1\)H NMR and IR) suggested that this compound was a sulfone, (1), rather than the isomeric sulfinate ester, (5). The X-ray crystal structure determination of (1), reported here, confirmed this structural assignment. Compound (1) crystallizes as discrete molecular species with the molecule comprising the asymmetric unit (Fig. 1). The bond lengths and angles are in accord with conventional values (Allen et al., 1987). The \( \text{CH}_2\text{COC}_2\text{H}_4\text{Br} \) fragment is essentially planar, with the \( \text{C}_4-\text{S}_1 \) bond lying nearly...
perpendicular to this plane, with $S_1-C_4-C_5-O_3 = -91.4(7)$.

**Experimental**

The title compound was prepared according to published procedures (Hiscock et al., 1995). Crystals suitable for X-ray diffraction studies were obtained as pale-yellow needles by recrystallization from ethanol (m.p. 401–403 K).

**Crystal data**

$\text{C}_{11}\text{H}_{11}\text{BrO}_3\text{S}$  
$M_r = 303.17$

Triclinic, $\text{P} \bar{1}$  
$\alpha = 5.2688(13)$ Å  
$\beta = 8.5968(11)$ Å  
$\gamma = 13.878(2)$ Å  
$\alpha = 74.393(10)^\circ$  
$\beta = 89.598(18)^\circ$  
$\gamma = 88.870(16)^\circ$  
$V = 670.37(19)$ Å$^3$

$\text{Mr} = 8.5968(11)$ Å

$\text{D}_r = 1.658 \text{Mg m}^{-3}$

Mo $\text{K}\alpha$ radiation  
Cell parameters from 25 standard reflections

$\theta = 11.9-15.9^\circ$  
$\mu = 3.54 \text{mm}^{-1}$  
$T = 295(2)$ K  
Needle, pale yellow  
$0.25 \times 0.10 \times 0.04$ mm

$Z = 2$

$R_{	ext{max}} = 0.030$

$\theta_{\text{max}} = 25.0^\circ$

$h = -6 \rightarrow 6$

$k = 0 \rightarrow 10$

$l = -15 \rightarrow 16$

3 standard reflections every 150 reflections

$wR_{\text{max}} = 0.29 \text{e Å}^{-3}$

$\Delta \rho_{\text{min}} = -0.29 \text{e Å}^{-3}$

$R_{1} = 0.034$

$wR_{2} = 0.088$

$S = 1.02$

2142 reflections

145 parameters

**Table 1**

Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>Bond</th>
<th>Length (Å)</th>
<th>Angle (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Br1–C9</td>
<td>1.895 (4)</td>
<td>C1–C2</td>
</tr>
<tr>
<td>S1–O1</td>
<td>1.430 (4)</td>
<td>C2–C3</td>
</tr>
<tr>
<td>S1–O2</td>
<td>1.435 (3)</td>
<td>C4–C5</td>
</tr>
<tr>
<td>S1–C3</td>
<td>1.778 (5)</td>
<td>C5–C6</td>
</tr>
<tr>
<td>S1–C4</td>
<td>1.774 (4)</td>
<td>C6–C7</td>
</tr>
<tr>
<td>O3–C5</td>
<td>1.211 (5)</td>
<td></td>
</tr>
<tr>
<td>O1–S1–O2</td>
<td>117.4 (2)</td>
<td>S1–C3–C2</td>
</tr>
<tr>
<td>O1–S1–C3</td>
<td>108.5 (2)</td>
<td>S1–C4–C5</td>
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<td>O1–S1–C4</td>
<td>108.7 (2)</td>
<td>O3–C5–C4</td>
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<tr>
<td>O2–S1–C3</td>
<td>109.0 (2)</td>
<td>O5–C5–C6</td>
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<td>O2–S1–C4</td>
<td>108.5 (2)</td>
<td>C4–C5–C6</td>
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<tr>
<td>C3–S1–C4</td>
<td>104.0 (2)</td>
<td>Br1–C9–C8</td>
</tr>
<tr>
<td>C1–C2–C3</td>
<td>126.8 (6)</td>
<td>Br1–C9–C10</td>
</tr>
</tbody>
</table>

**Figure 1**

View of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. H atoms are included as spheres of arbitrary radii.

H atoms were constrained as riding atoms, fixed to their parent C atoms at a C–H distance of 0.95 Å. $U_{	ext{iso}}$(H) values were set at 1.2$U_{	ext{eq}}$ of the parent atom.

Data collection: MSC/AFC-7 Diffractometer Control Software (Molecular Structure Corporation, 1999); cell refinement: MSC/AFC-7 Diffractometer Control Software; data reduction: TEXSAN for Windows (Molecular Structure Corporation, 2001); program(s) used to solve structure: TEXSAN for Windows; program(s) used to refine structure: TEXSAN for Windows and SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: TEXSAN for Windows and PLATON (Spek, 2003).

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**References**


