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1-(4-Bromophenyl)-2-(2-propenylsulfonyl)-ethanone

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The title compound, $C_{11}H_{11}BrO_3S$, was prepared by reaction of sodium allylsulfinate with *p*-bromophenacyl bromide to confirm the identity of the former.

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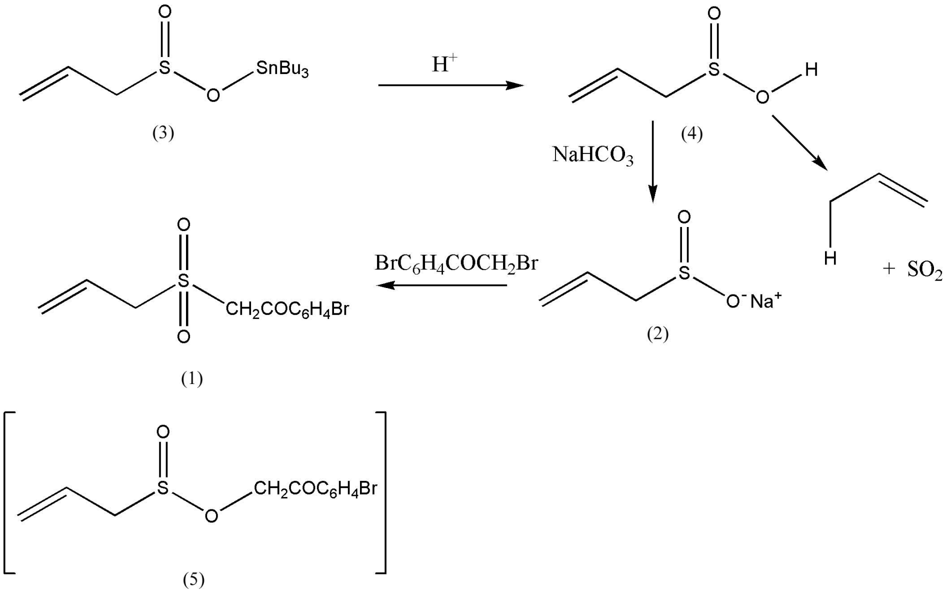
Key indicators

Single-crystal X-ray study
T = 295 K
Mean *σ*(C–C) = 0.007 Å
R factor = 0.034
wR factor = 0.088
Data-to-parameter ratio = 14.8

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

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 tributylltin 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 $CH_2COC_6H_4Br$ fragment is essentially planar, with the C4—S1 bond lying nearly perpendicular to this plane, with S1—C4—C5—O3 = −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

$C_{11}H_{11}BrO_3S$
$M_r = 303.17$
Triclinic, $P\overline{1}$
$a = 5.2868\ (13)$ Å
$b = 8.5968\ (11)$ Å
$c = 13.878\ (2)$ Å
$\alpha = 74.393\ (10)^\circ$
$\beta = 89.598\ (18)^\circ$
$\gamma = 88.870\ (16)^\circ$
$V = 607.37\ (19)$ Å^3

$Z = 2$
$D_x = 1.658$ Mg m^{-3}
Mo Kα radiation
Cell parameters from 25 reflections
$\theta = 11.9$–15.9°
$\mu = 3.54$ mm^{-1}
$T = 295\ (2)$ K
Needle, pale yellow
$0.25 \times 0.10 \times 0.04$ mm

Data collection

Rigaku AFC-7*R* diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.471$, $T_{\max} = 0.871$
2298 measured reflections
2142 independent reflections
1185 reflections with $I > 2\sigma(I)$

$R_{\rm int} = 0.030$
$\theta_{\max} = 25.0^\circ$
$h = -6 \rightarrow 6$
$k = 0 \rightarrow 10$
$l = -15 \rightarrow 16$
3 standard reflections every 150 reflections intensity decay: 1.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.088$
$S = 1.02$
2142 reflections
145 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0259P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.29$ e Å^{-3}
$\Delta\rho_{\min} = -0.29$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—C9	1.895 (4)	C1—C2	1.236 (11)
S1—O1	1.430 (4)	C2—C3	1.492 (9)
S1—O2	1.435 (3)	C4—C5	1.522 (6)
S1—C3	1.778 (5)	C5—C6	1.485 (6)
S1—C4	1.774 (4)	C6—C7	1.386 (6)
O3—C5	1.211 (5)		
O1—S1—O2	117.4 (2)	S1—C3—C2	112.8 (4)
O1—S1—C3	108.5 (2)	S1—C4—C5	111.0 (3)
O1—S1—C4	108.7 (2)	O3—C5—C4	118.7 (4)
O2—S1—C3	109.0 (2)	O3—C5—C6	122.0 (4)
O2—S1—C4	108.5 (2)	C4—C5—C6	119.4 (4)
C3—S1—C4	104.0 (2)	Br1—C9—C8	119.6 (3)
C1—C2—C3	126.8 (6)	Br1—C9—C10	118.9 (3)

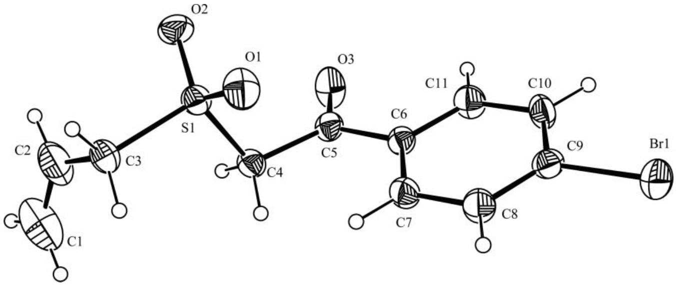


Figure 1
View of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. H atoms are included as spheres of arbitrary radii.

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