Table 2. *Bond lengths* (Å) *and angles* (°)

C(1)—O(2)	1·419 (3)	C(1)—C(7a)	1·518 (3)
C(1)—O(16)	1·421 (2)	O(2)—C(3)	1·352 (3)
C(3)—C(4)	1·324 (3)	C(4)—C(4a)	1·505 (3)
C(4)—C(12)	1·467 (3)	C(4a)—C(5)	1·526 (3)
C(4a)—C(7a)	1·533 (3)	C(5)—C(6)	1·522 (4)
C(6)—C(7)	1·517 (3)	C(7)—C(7a)	1·535 (3)
C(7a)—O(8)	1·464 (2)	O(8)—C(9)	1·348 (2)
C(9)—C(10)	1·484 (3)	C(9)—O(11)	1·205 (3)
C(12)—O(13)	1·339 (3)	C(12)—O(15)	1·202 (3)
O(13)—C(14)	1·435 (3)	O(16)—C(17)	1·353 (3)
C(17)—C(18)	1·492 (4)	C(17)—O(19)	1·186 (3)

O(2)—C(1)—C(7a)	110·5 (2)	O(2)—C(1)—O(16)	109·1 (2)
C(7a)—C(1)—O(16)	106·7 (2)	C(1)—O(2)—C(3)	115·4 (2)
O(2)—C(3)—C(4)	125·8 (2)	C(3)—C(4)—C(4a)	122·0 (2)
C(3)—C(4)—C(12)	116·7 (2)	C(4a)—C(4)—C(12)	121·3 (2)
C(4)—C(4a)—C(5)	111·6 (2)	C(4)—C(4a)—C(7a)	109·3 (2)
C(5)—C(4a)—C(7a)	102·3 (2)	C(4a)—C(5)—C(6)	103·7 (2)
C(5)—C(6)—C(7)	105·3 (2)	C(6)—C(7)—C(7a)	106·4 (2)
C(1)—C(7a)—C(4a)	112·3 (2)	C(1)—C(7a)—C(7)	113·7 (2)
C(4a)—C(7a)—C(7)	105·8 (2)	C(1)—C(7a)—O(8)	109·2 (2)
C(4a)—C(7a)—O(8)	103·6 (1)	C(7)—C(7a)—O(8)	111·7 (2)
C(7a)—O(8)—C(9)	120·0 (1)	O(8)—C(9)—C(10)	111·4 (2)
O(8)—C(9)—O(11)	123·7 (2)	C(10)—C(9)—O(11)	124·8 (2)
C(4)—C(12)—O(13)	112·6 (2)	C(4)—C(12)—O(15)	125·8 (2)
O(13)—C(12)—O(15)	121·7 (2)	C(12)—O(13)—C(14)	116·2 (2)
C(1)—O(16)—C(17)	117·5 (2)	O(16)—C(17)—C(18)	110·4 (2)
O(16)—C(17)—O(19)	122·6 (2)	C(18)—C(17)—O(19)	127·0 (2)

Fig. 1. The asymmetric unit of the title compound, showing the atom-numbering scheme.

Related literature. For the preparation of the compound see Zimmermann (1980). For the structure of the iridoid compound loganin see Jones, Sheldrick, Glüsenkamp & Tietze (1980).

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Structure of a Cycloheptenone Derivative

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Abstract. Racemic (1R,7S,9R)-2-methyl-6-oxobicyclo-[5.3.0]dec-2-en-9-yl methanesulfonate, $C_{12}H_{18}O_4S$, $M_r = 258\cdot3$, orthorhombic, *Pbca*, $a = 8\cdot745$ (2), $b = 33\cdot451$ (5), $c = 8\cdot845$ (2) Å, $V = 2588$ Å^3, $Z = 8$, $D_x = 1\cdot326$ Mg m^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 0\cdot24$ mm^{-1}, $F(000) = 1104$, $T = 298$ K, $R = 0\cdot049$ for 1387 unique observed reflections. The seven-membered ring adopts a boat and the five-membered ring a half-chair conformation; the ring junction is *cis* and the mesyloxy group axial. It had not proved possible to
assign the conformation unambiguously from NMR data because of the difficulty in applying correlations to relatively flexible five- and seven-membered rings.

Experimental. (I): crystal $0\cdot3 \times 0\cdot3 \times 0\cdot4$ mm. Stoe–Siemens four-circle diffractometer, monochromated Mo $K\alpha$ radiation, profile-fitting mode involving variable scan width and speed (Clegg, 1981). 2064 reflections, $2\theta_{max}$ 45°, $+h+k+l$ and some $-h+k+l$, three check reflections with no intensity change. 1680 unique
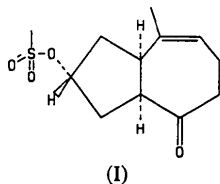
Table 1. *Atomic coordinates* $(\times 10^4)$ *and equivalent isotropic thermal parameters* $(\text{Å}^2 \times 10^3)$

	x	y	z	U_{eq}*
C(1)	1589 (4)	6332 (1)	4918 (4)	48 (1)
C(2)	1615 (4)	6416 (1)	3237 (4)	55 (1)
C(3)	2034 (4)	6757 (1)	2604 (4)	72 (1)
C(4)	2482 (6)	7133 (1)	3390 (5)	84 (2)
C(5)	1187 (5)	7308 (1)	4314 (5)	80 (2)
C(6)	472 (4)	7014 (1)	5383 (4)	53 (1)
C(7)	1477 (4)	6693 (1)	6035 (3)	48 (1)
C(8)	863 (4)	6517 (1)	7503 (4)	67 (1)
C(9)	324 (4)	6095 (1)	7149 (4)	59 (1)
C(10)	288 (4)	6067 (1)	5449 (4)	59 (1)
C(11)	1193 (6)	6066 (1)	2245 (5)	93 (2)
O(12)	−875 (3)	7031 (1)	5688 (3)	82 (1)
O(13)	1509 (2)	5821 (1)	7742 (3)	60 (1)
S(14)	1079 (1)	5435 (1)	8644 (1)	49 (1)
O(15)	−313 (3)	5497 (1)	9437 (3)	63 (1)
O(16)	2422 (3)	5348 (1)	9474 (3)	69 (1)
C(17)	804 (5)	5075 (1)	7275 (4)	73 (1)

* U_{eq} defined as one third of the trace of the orthogonalized U_{ij} tensor.

Fig. 1. The asymmetric unit of the title compound, showing the atom-numbering scheme.

Table 2. *Bond lengths* (Å) *and angles* (°)

C(1)—C(2)	1·513 (5)	C(1)—C(7)	1·565 (4)
C(1)—C(10)	1·516 (5)	C(2)—C(3)	1·324 (5)
C(2)—C(11)	1·508 (5)	C(3)—C(4)	1·489 (5)
C(4)—C(5)	1·513 (6)	C(5)—C(6)	1·500 (5)
C(6)—C(7)	1·502 (4)	C(6)—O(12)	1·210 (4)
C(7)—C(8)	1·524 (5)	C(8)—C(9)	1·519 (5)
C(9)—C(10)	1·507 (5)	C(9)—O(13)	1·479 (4)
O(13)—S(14)	1·564 (2)	S(14)—O(15)	1·420 (2)
S(14)—O(16)	1·416 (3)	S(14)—C(17)	1·725 (4)

C(2)—C(1)—C(7)	118·5 (3)	C(2)—C(1)—C(10)	115·1 (3)
C(7)—C(1)—C(10)	102·0 (2)	C(1)—C(2)—C(3)	125·5 (3)
C(1)—C(2)—C(11)	115·1 (3)	C(3)—C(2)—C(11)	119·4 (3)
C(2)—C(3)—C(4)	127·1 (3)	C(3)—C(4)—C(5)	112·4 (4)
C(4)—C(5)—C(6)	113·6 (3)	C(5)—C(6)—C(7)	117·7 (3)
C(5)—C(6)—O(12)	121·1 (3)	C(7)—C(6)—O(12)	121·1 (3)
C(1)—C(7)—C(6)	110·3 (2)	C(1)—C(7)—C(8)	105·1 (2)
C(6)—C(7)—C(8)	113·4 (3)	C(7)—C(8)—C(9)	107·1 (3)
C(8)—C(9)—C(10)	105·6 (3)	C(8)—C(9)—O(13)	106·6 (3)
C(10)—C(9)—O(13)	109·3 (3)	C(1)—C(10)—C(9)	104·9 (3)
C(9)—O(13)—S(14)	121·6 (2)	O(13)—S(14)—O(15)	109·7 (1)
O(13)—S(14)—O(16)	103·6 (1)	O(15)—S(14)—O(16)	119·0 (1)
O(13)—S(14)—C(17)	104·6 (2)	O(15)—S(14)—C(17)	109·2 (2)
O(16)—S(14)—C(17)	109·6 (2)		

Structure solution by multisolution direct methods. Refinement on F to $R = 0·049$, $wR = 0·059$; all non-H atoms anisotropic, H atoms included using a riding model [C—H 0·96 Å, $U(\text{H}) = 1·2U_{eq}(\text{C})$], 160 parameters, $S = 1·49$, weighting scheme $w^{-1} = \sigma^2(F) + 0·00072F^2$ which gave a featureless analysis of variance in terms of $\sin\theta$ and F_o, max. $\Delta/\sigma = 0·06$, max. and min. height in final $\Delta\rho$ map 0·24 and −0·30 e Å^{-3} respectively. Atomic scattering factors from *SHELXTL*.

Atomic parameters are given in Table 1, bond distances and angles in Table 2.* Fig. 1 shows the atom numbering.

Related literature. For the preparation of the compound see Reichert (1985). For a related structure with *cis*-fused five- and seven-membered rings see Rychlewska (1985).

(I)

reflections ($R_{int} = 0·061$), of which 1387 with $F > 3\sigma(F)$ used for all calculations (program system *SHELXTL*, Sheldrick, 1978). Index range $|h| \le 9$, $k \le 36$, $l \le 9$. Cell constants refined from $\pm 2\theta$ values of 36 reflections in range 20–25°. Absorption and extinction corrections unnecessary.
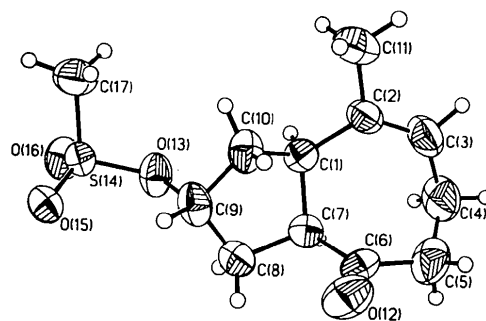
* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43130 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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