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# 2-Phenyl-*N*-(*p*-tolylsulfonyl)aziridine

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**Key indicators**

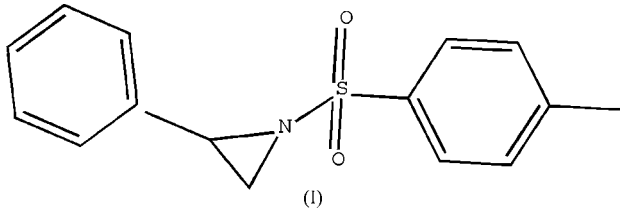
Single-crystal X-ray study
$T$ = 294 K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.043
$wR$ factor = 0.118
Data-to-parameter ratio = 15.6

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

The title compound, $C_{15}H_{15}NO_2S$, is an aziridination product of styrene formed using chloramine-T as a substrate. In the molecule, the aziridine ring is nearly perpendicular to the adjacent aromatic ring.

## Comment

The aziridination of olefins using chloramine-T as the nitrogen source (Jeong *et al.*, 1998) is a practical method (Thakur & Sudalai, 2003) widely used in the synthesis of aziridines. We have recently prepared the title compound, (I), by this method and report its crystal structure here.




(I)

The molecular structure of (I) is shown in Fig. 1. In the molecule, the two aromatic rings form a dihedral angle of 112.2 (1)°, and the aziridine ring is nearly perpendicular to the adjacent phenyl ring, with a dihedral angle of 88.4 (1)°. The dihedral angle between the aziridine ring and the *p*-tolyl ring is 23.9 (1)°.

## Experimental

Anhydrous chloramine-T (12.5 g) and *N*-bromosuccinamide (2.0 g) were dissolved in anhydrous acetonitrile (250 ml) and then freshly distilled styrene (5.0 g) was slowly added. The resulting mixture was stirred at room temperature for 12 h (monitored by thin-layer chromatography). The reaction mixture was then diluted with EtOAc (50 ml) and washed successively with water and brine. The organic layer was dried over anhydrous $MgSO_4$ and concentrated under reduced pressure to afford a crude product that was purified by column chromatography on silica gel using petroleum ether and EtOAc in the proportion of 6:1 as the eluent to afford colorless crystals of (I) (yield 63%). These crystals melted at 362 K.

*Crystal data*

$C_{15}H_{15}NO_2S$
$M_r$ = 273.34
Monoclinic, $P2_1/c$
$a$ = 15.325 (3) Å
$b$ = 7.8364 (16) Å
$c$ = 11.773 (2) Å
$\beta$ = 93.293 (4)°
$V$ = 1411.5 (5) Å$^3$
$Z$ = 4
$D_x$ = 1.286 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 2001 reflections
$\theta$ = 2.9–22.6°
$\mu$ = 0.23 mm$^{-1}$
$T$ = 294 (2) K
Block, colourless
0.30 × 0.24 × 0.20 mm

*Data collection*

Bruker SMART CCD area detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.935, $T_{max}$ = 0.956
7714 measured reflections
2893 independent reflections
1663 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041
$\theta_{max}$ = 26.4°
$h = -19 \rightarrow 8$
$k = -9 \rightarrow 9$
$l = -14 \rightarrow 14$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.118
$S$ = 1.01
2893 reflections
185 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0652P)^2 + 0.0807P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| S1—O1 | 1.4250 (17) | S1—C9 | 1.745 (2) |
| S1—O2 | 1.4293 (16) | N1—C8 | 1.476 (3) |
| S1—N1 | 1.6589 (17) | N1—C7 | 1.497 (3) |
| | | | |
| O1—S1—O2 | 117.98 (11) | C8—C7—N1 | 60.00 (17) |
| N1—S1—C9 | 100.92 (9) | C7—C8—N1 | 61.41 (16) |
| C8—N1—C7 | 58.59 (17) | | |

H atoms on the three-membered ring were located in a difference map and refined freely with isotropic displacement parameters. All other H atoms were positioned geometrically (C—H = 0.88–0.96 Å) and refined as riding. $U_{iso}$(H) values were set to $1.2U_{eq}$(carrier atom) except for the methyl groups where they were set to $1.5U_{eq}$(carrier atom).

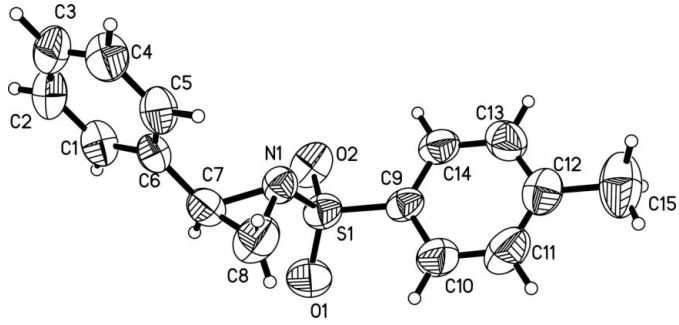



**Figure 1**
View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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