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# 4-*tert*-Butylphenyl 4-methylbenzenesulfonate

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In the title compound, $C_{17}H_{20}O_3S$, the dihedral angle between the planes of the two aromatic rings is 66.5 (1)°. Weak C—H···O interactions are observed in the crystal structure.

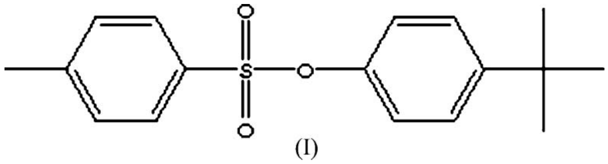
**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean $\sigma$(C–C) = 0.004 Å
*R* factor = 0.060
*wR* factor = 0.182
Data-to-parameter ratio = 19.6

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

## Comment

Aromatic sulfonates can serve as important materials in detecting specific organic anion binding proteins in the liver plasma membrane (Yachi *et al.*, 1989), as well as in many other fields (Narayanan & Krakow, 1983; Jiang *et al.*, 1990; Alford *et al.*, 1991; Tharakan *et al.*, 1992; Spungin *et al.*, 1992). The crystal structures of several aromatic sulfonates have been reported (Vembu *et al.*, 2004*a*,*b*). However, the structures of alkyl-substituted aromatic sulfonates have not been studied. Therefore, we have undertaken an X-ray crystal structure analysis of the title compound, (I). This study may serve as a forerunner both for an assessment of the biological significance of this compound and for study of the structural features influencing its activity.



(I)

The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. The bond lengths and angles in (I) are normal. The S1—O3 bond is slightly longer than the corresponding bond in other sulfonates [1.579 (3) and 1.589 (4)Å; Vembu *et al.*, 2004*a*,*b*]. The dihedral angle between the planes of the two aromatic rings is 66.5 (1)°. These rings have a non-coplanar orientation, similar to that reported for other aromatic sulfonates (Vembu *et al.*, 2004*a*,*b*) and in contrast to the near-coplanar orientation found in 4-methoxyphenyl 4-toluenesulfonate (Vembu, Nallu, Garrison, Hindi & Youngs, 2003), 2,4-dinitrophenyl 4-toluenesulfonate (Vembu, Nallu, Garrison & Youngs, 2003) and 8-quinolyl 3-nitrobenzenesulfonate (Vembu, Nallu, Spencer & Howard, 2003).

The crystal structure of (I) is stabilized by weak C—H···O interactions (Table 2). The C2—H2···O1 and C2—H2···O2 interactions constitute a pair of bifurcated donor bonds.

## Experimental

The title compound was prepared by the addition of a solution of tosyl chloride (1.90 g, 10 mmol) dissolved in acetone (10 ml) to a solution of *p*-*tert*-butylphenol (10 mmol) dissolved in NaOH (8 ml, 5%). The precipitated solid (2.47 g, 8.1 mmol, yield 81%; m.p. 370–371 K) was recrystallized from an acetone–ethanol (1:1) solution.

*Crystal data*

$C_{17}H_{20}O_3S$
$M_r = 304.39$
Monoclinic, $P2_1/c$
$a = 11.557$ (2) Å
$b = 12.611$ (3) Å
$c = 11.858$ (2) Å
$\beta = 105.80$ (3)°
$V = 1662.9$ (6) Å$^3$
$Z = 4$
$D_x = 1.216$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.20$ mm$^{-1}$
$T = 293$ (2) K
Block, colourless
0.79 × 0.56 × 0.45 mm

*Data collection*

Rigaku R-AXIS RAPID imaging-plate diffractometer
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.857$, $T_{\max} = 0.915$
11643 measured reflections
3747 independent reflections
2344 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.056$
$\theta_{\max} = 27.5°$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.182$
$S = 1.00$
3747 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0998P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.010$
$\Delta\rho_{\max} = 0.45$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.38$ e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| S1—O1 | 1.418 (2) | O3—C8 | 1.424 (2) |
| S1—O2 | 1.4246 (19) | C4—C7 | 1.492 (4) |
| S1—O3 | 1.5958 (17) | C11—C14 | 1.528 (3) |
| S1—C1 | 1.737 (3) | | |
| O1—S1—O2 | 120.12 (13) | C13—C8—O3 | 118.0 (2) |
| O1—S1—O3 | 102.26 (12) | C10—C11—C12 | 116.7 (2) |
| O2—S1—O3 | 109.40 (10) | C10—C11—C14 | 122.2 (2) |
| O1—S1—C1 | 110.64 (13) | C12—C11—C14 | 121.0 (2) |
| O2—S1—C1 | 109.78 (12) | C13—C12—C11 | 122.2 (2) |
| O3—S1—C1 | 103.05 (10) | C15—C14—C11 | 112.5 (2) |
| C8—O3—S1 | 119.81 (13) | C17—C14—C11 | 111.0 (2) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C2—H2···O2 | 0.93 | 2.53 | 2.903 (3) | 104 |
| C2—H2···O1$^{\rm i}$ | 0.93 | 2.59 | 3.230 (3) | 126 |
| C6—H6···O3$^{\rm ii}$ | 0.93 | 2.59 | 3.478 (4) | 161 |

Symmetry codes: (i) $x, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $-x+2, -y, -z+1$.

H atoms were placed in idealized positions and allowed to ride on their respective parent atoms, with C—H distances in the range 0.93–0.96Å, and with $U_{\rm iso}({\rm H}) = 1.2$–$1.5U_{\rm eq}({\rm C})$.

Data collection: *RAPID-AUTO* (Rigaku 2003); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

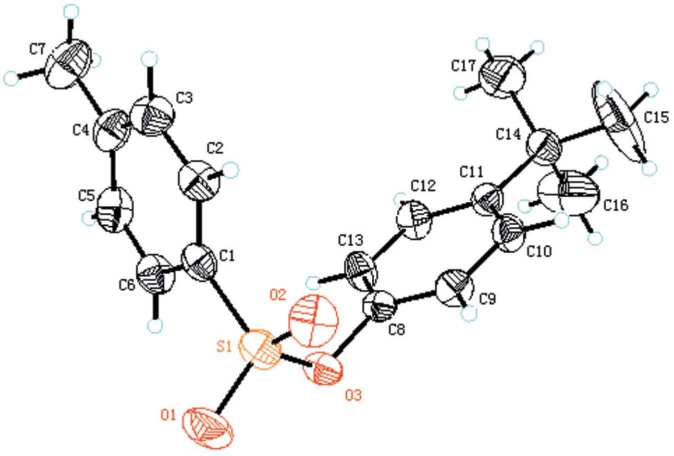


**Figure 1**
The molecular structure of (I), showing the atom-labelling scheme and 40% probability displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii.

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