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2-Ethoxy-4-methylphenyl *p*-toluenesulfonate

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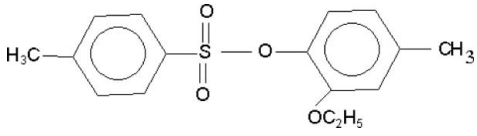
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.106; data-to-parameter ratio = 13.8.

In the title compound, $C_{16}H_{18}O_4S$, the dihedral angle between the two aromatic rings is 43.71 (6)°. The molecular structure is stabilized by a weak intramolecular C–H···O interaction and the crystal packing is stabilized by weak intermolecular C—H···O interactions.

Related literature

For related literature, see: Manivannan *et al.* (2005*a*); Spungin *et al.* (1984); Yachi *et al.* (1989). A similar compound has been reported by Manivannan *et al.* (2005*b*).



Experimental

Crystal data

$C_{16}H_{18}O_4S$
M_r = 306.36
Triclinic, $P\overline{1}$
a = 7.8095 (10) Å
b = 9.2787 (12) Å
c = 11.4058 (15) Å
α = 104.678 (2)°
β = 99.653 (2)°
γ = 94.906 (2)°
V = 781.06 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 295 (2) K
0.48 × 0.46 × 0.14 mm

Data collection

Bruker Kappa APEX2 diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.902, T_{max} = 0.970
7352 measured reflections
2654 independent reflections
2338 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.107
S = 1.06
2654 reflections
193 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O3	0.93	2.57	2.926 (2)	103
C2—H2···O1^{i}	0.93	2.58	3.353 (2)	141
C12—H12···O3^{ii}	0.93	2.48	3.310 (2)	149

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+1, -y, -z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2585).

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supplementary materials

Acta Cryst. (2007). E**63**, o4638 [**doi:10.1107/S160053680705619X**]

2-Ethoxy-4-methylphenyl *p*-toluenesulfonate

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Comment

Several compounds containing the *para*-toluene sulfonate moiety are used in the fields of biology and industry. The merging of lipids can be monitored using a derivative of *para*-toluene sulfonate (Yachi *et al.*, 1989). This method has been used in studying the membrane fusion during the acrosome reaction (Spungin *et al.*, 1984).

The geometric parameters in the title compound (Fig. 1) agree with the reported values of similar structures (Manivannan *et al.*, 2005*a*; Manivannan *et al.*, 2005*b*). The dihedral angle between the two phenyl rings is 43.71 (6)°. The ethoxy group is almost coplanar with the benzene ring C18—C13 to which it attached, with the dihedral angle of 4.84 (10)°.

The details of the hydrogen bonding are given in Table 1. The molecular structure is stabilized by a weak intramolecular C—H···O interaction and the crystal packing (Fig. 2) is stabilized by weak intermolecular C—H···O interactions.

Experimental

2-ethoxy, 4 methyl phenol (4.9 mmol)(17), triethylamine (4.9 mmol), were dissolved separately in acetone (10 ml) and mixed. To this solution, 4-toluene sulfonyl chloride (3.9 mmol), dissolved in acetone (10 ml) was added. The solution was left overnight and evaporated. The residue obtained was washed several times with 2% aqueous triethylamine solution to obtain the crude product. Crystals were obtained by recrystallizing the crude product (2.6 mmol, 68% yield) from ethanol.

Refinement

H atoms were positioned geometrically and refined using riding model with C—H = 0.93 Å and U_{iso}(H) = 1.2Ueq(C) for aromatic C—H, C—H = 0.97 Å and U_{iso}(H) = 1.2Ueq(C) for CH_2 and C—H = 0.96 Å and U_{iso}(H) = 1.5Ueq(C) for CH_3.

Figures

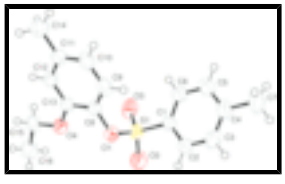

Fig. 1. The molecular structure of the title compound, with atom labels and 50% probability displacement ellipsoids for non-H atoms.

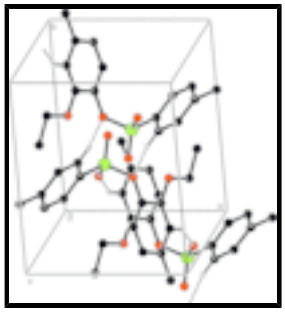

Fig. 2. The packing of the title compound, viewed down the *c* axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

2-Ethoxy-4-methylphenyl *p*-toluenesulfonate

Crystal data

$C_{16}H_{18}O_4S$	$Z = 2$
$M_r = 306.36$	$F_{000} = 324$
Triclinic, $P\overline{1}$	$D_x = 1.303$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.8095$ (10) Å	Cell parameters from 2654 reflections
$b = 9.2787$ (12) Å	$\theta = 1.9$–24.7°
$c = 11.4058$ (15) Å	$\mu = 0.22$ mm^{-1}
$\alpha = 104.678$ (2)°	$T = 295$ (2) K
$\beta = 99.653$ (2)°	Block, colourless
$\gamma = 94.906$ (2)°	0.48 × 0.46 × 0.14 mm
$V = 781.06$ (18) Å^3	

Data collection

Bruker Kappa APEX) diffractometer	2654 independent reflections
Radiation source: fine-focus sealed tube	2338 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.016$
$T = 295$(2) K	$\theta_{max} = 24.7^\circ$
ω and φ scan	$\theta_{min} = 1.9^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -9 \rightarrow 9$
$T_{min} = 0.902$, $T_{max} = 0.970$	$k = -10 \rightarrow 10$
7352 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.039$	H-atom parameters constrained
$wR(F^2) = 0.107$	$w = 1/[\sigma^2(F_o^2) + (0.0551P)^2 + 0.2034P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
2654 reflections	$\Delta\rho_{max}$ = 0.21 e Å^{-3}
193 parameters	$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.34100 (7)	0.33058 (5)	0.26424 (4)	0.05261 (18)
O1	0.52497 (16)	0.28192 (14)	0.31438 (12)	0.0548 (4)
O4	0.69333 (17)	0.21268 (14)	0.12633 (12)	0.0544 (4)
O3	0.2656 (2)	0.23076 (18)	0.14687 (12)	0.0674 (4)
O2	0.3812 (2)	0.48652 (17)	0.27924 (16)	0.0795 (5)
C1	0.2133 (2)	0.3036 (2)	0.37126 (16)	0.0440 (4)
C13	0.6426 (2)	0.0974 (2)	0.17164 (15)	0.0435 (4)
C12	0.6741 (2)	−0.0497 (2)	0.12995 (16)	0.0464 (4)
H12	0.7323	−0.0753	0.0643	0.056*
C8	0.5536 (2)	0.1316 (2)	0.26945 (16)	0.0455 (4)
C9	0.5040 (2)	0.0247 (2)	0.32517 (17)	0.0538 (5)
H9	0.4477	0.0506	0.3918	0.065*
C6	0.0909 (2)	0.1766 (2)	0.34244 (17)	0.0517 (5)
H6	0.0768	0.1046	0.2669	0.062*
C15	0.7938 (3)	0.1811 (2)	0.03069 (18)	0.0528 (5)
H15A	0.7230	0.1125	−0.0438	0.063*
H15B	0.8951	0.1350	0.0567	0.063*
C11	0.6209 (2)	−0.1601 (2)	0.18391 (18)	0.0493 (4)
C2	0.2360 (3)	0.4108 (2)	0.48349 (17)	0.0522 (5)
H2	0.3187	0.4958	0.5024	0.063*
C4	0.0098 (3)	0.2646 (2)	0.54036 (19)	0.0559 (5)
C10	0.5370 (3)	−0.1207 (2)	0.28299 (18)	0.0566 (5)
H10	0.5030	−0.1929	0.3211	0.068*
C5	−0.0096 (3)	0.1585 (2)	0.42711 (19)	0.0566 (5)
H5	−0.0922	0.0735	0.4081	0.068*
C3	0.1343 (3)	0.3898 (2)	0.56696 (18)	0.0611 (5)
H3	0.1496	0.4612	0.6429	0.073*
C14	0.6526 (3)	−0.3197 (2)	0.1314 (2)	0.0688 (6)
H14A	0.5991	−0.3841	0.1728	0.103*
H14B	0.7764	−0.3245	0.1432	0.103*
H14C	0.6025	−0.3521	0.0446	0.103*
C16	0.8511 (3)	0.3271 (3)	0.0064 (2)	0.0790 (7)
H16A	0.7499	0.3713	−0.0199	0.118*
H16B	0.9193	0.3094	−0.0572	0.118*
H16C	0.9208	0.3941	0.0807	0.118*
C7	−0.1038 (4)	0.2435 (3)	0.6305 (3)	0.0897 (8)
H7A	−0.0548	0.1789	0.6772	0.135*
H7B	−0.2196	0.1988	0.5862	0.135*
H7C	−0.1096	0.3393	0.6858	0.135*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0591 (3)	0.0523 (3)	0.0535 (3)	0.0119 (2)	0.0268 (2)	0.0154 (2)
O1	0.0466 (7)	0.0511 (8)	0.0602 (8)	0.0028 (6)	0.0201 (6)	−0.0012 (6)
O4	0.0615 (8)	0.0459 (7)	0.0635 (8)	0.0069 (6)	0.0322 (7)	0.0160 (6)
O3	0.0696 (9)	0.0892 (11)	0.0448 (8)	0.0208 (8)	0.0181 (7)	0.0129 (7)
O2	0.0996 (12)	0.0575 (9)	0.1041 (12)	0.0188 (8)	0.0587 (10)	0.0346 (9)
C1	0.0412 (9)	0.0472 (10)	0.0467 (10)	0.0100 (8)	0.0151 (8)	0.0127 (8)
C13	0.0392 (9)	0.0470 (10)	0.0428 (9)	0.0001 (7)	0.0108 (7)	0.0099 (8)
C12	0.0465 (10)	0.0497 (11)	0.0441 (10)	0.0059 (8)	0.0160 (8)	0.0102 (8)
C8	0.0379 (9)	0.0488 (10)	0.0459 (10)	0.0019 (8)	0.0120 (8)	0.0047 (8)
C9	0.0471 (10)	0.0686 (13)	0.0499 (11)	0.0064 (9)	0.0212 (8)	0.0163 (9)
C6	0.0513 (11)	0.0516 (11)	0.0484 (10)	0.0031 (8)	0.0109 (8)	0.0073 (8)
C15	0.0521 (11)	0.0580 (12)	0.0553 (11)	0.0079 (9)	0.0232 (9)	0.0196 (9)
C11	0.0453 (10)	0.0488 (11)	0.0547 (11)	0.0042 (8)	0.0110 (8)	0.0156 (8)
C2	0.0546 (11)	0.0475 (11)	0.0528 (11)	0.0027 (8)	0.0180 (9)	0.0069 (9)
C4	0.0520 (11)	0.0659 (13)	0.0631 (12)	0.0203 (10)	0.0250 (9)	0.0287 (10)
C10	0.0530 (11)	0.0627 (13)	0.0638 (12)	0.0053 (9)	0.0218 (10)	0.0286 (10)
C5	0.0427 (10)	0.0614 (12)	0.0693 (13)	0.0023 (9)	0.0132 (9)	0.0242 (10)
C3	0.0736 (14)	0.0638 (13)	0.0479 (11)	0.0171 (11)	0.0243 (10)	0.0080 (9)
C14	0.0793 (15)	0.0508 (12)	0.0835 (15)	0.0122 (11)	0.0262 (12)	0.0230 (11)
C16	0.0830 (17)	0.0744 (16)	0.0989 (18)	0.0104 (12)	0.0454 (14)	0.0408 (14)
C7	0.0916 (18)	0.109 (2)	0.0970 (19)	0.0282 (16)	0.0599 (16)	0.0468 (16)

Geometric parameters (Å, °)

S1—O2	1.4143 (16)	C15—H15B	0.9700
S1—O3	1.4180 (15)	C11—C10	1.385 (3)
S1—O1	1.6004 (14)	C11—C14	1.509 (3)
S1—C1	1.7517 (17)	C2—C3	1.377 (3)
O1—C8	1.410 (2)	C2—H2	0.9300
O4—C13	1.358 (2)	C4—C3	1.384 (3)
O4—C15	1.434 (2)	C4—C5	1.388 (3)
C1—C2	1.381 (2)	C4—C7	1.504 (3)
C1—C6	1.384 (3)	C10—H10	0.9300
C13—C12	1.385 (2)	C5—H5	0.9300
C13—C8	1.395 (2)	C3—H3	0.9300
C12—C11	1.390 (3)	C14—H14A	0.9600
C12—H12	0.9300	C14—H14B	0.9600
C8—C9	1.369 (3)	C14—H14C	0.9600
C9—C10	1.375 (3)	C16—H16A	0.9600
C9—H9	0.9300	C16—H16B	0.9600
C6—C5	1.375 (3)	C16—H16C	0.9600
C6—H6	0.9300	C7—H7A	0.9600
C15—C16	1.496 (3)	C7—H7B	0.9600
C15—H15A	0.9700	C7—H7C	0.9600

O2—S1—O3	121.17 (10)	C12—C11—C14	119.16 (17)
O2—S1—O1	103.58 (9)	C3—C2—C1	118.89 (18)
O3—S1—O1	109.09 (8)	C3—C2—H2	120.6
O2—S1—C1	109.05 (9)	C1—C2—H2	120.6
O3—S1—C1	108.99 (9)	C3—C4—C5	118.35 (18)
O1—S1—C1	103.46 (8)	C3—C4—C7	121.4 (2)
C8—O1—S1	118.68 (11)	C5—C4—C7	120.3 (2)
C13—O4—C15	117.46 (14)	C9—C10—C11	120.26 (18)
C2—C1—C6	120.97 (17)	C9—C10—H10	119.9
C2—C1—S1	119.08 (14)	C11—C10—H10	119.9
C6—C1—S1	119.95 (14)	C6—C5—C4	121.28 (19)
O4—C13—C12	125.41 (15)	C6—C5—H5	119.4
O4—C13—C8	116.83 (16)	C4—C5—H5	119.4
C12—C13—C8	117.75 (16)	C2—C3—C4	121.48 (18)
C13—C12—C11	121.53 (16)	C2—C3—H3	119.3
C13—C12—H12	119.2	C4—C3—H3	119.3
C11—C12—H12	119.2	C11—C14—H14A	109.5
C9—C8—C13	121.27 (17)	C11—C14—H14B	109.5
C9—C8—O1	120.61 (16)	H14A—C14—H14B	109.5
C13—C8—O1	118.02 (16)	C11—C14—H14C	109.5
C8—C9—C10	120.21 (17)	H14A—C14—H14C	109.5
C8—C9—H9	119.9	H14B—C14—H14C	109.5
C10—C9—H9	119.9	C15—C16—H16A	109.5
C5—C6—C1	119.04 (18)	C15—C16—H16B	109.5
C5—C6—H6	120.5	H16A—C16—H16B	109.5
C1—C6—H6	120.5	C15—C16—H16C	109.5
O4—C15—C16	107.62 (16)	H16A—C16—H16C	109.5
O4—C15—H15A	110.2	H16B—C16—H16C	109.5
C16—C15—H15A	110.2	C4—C7—H7A	109.5
O4—C15—H15B	110.2	C4—C7—H7B	109.5
C16—C15—H15B	110.2	H7A—C7—H7B	109.5
H15A—C15—H15B	108.5	C4—C7—H7C	109.5
C10—C11—C12	118.93 (17)	H7A—C7—H7C	109.5
C10—C11—C14	121.89 (18)	H7B—C7—H7C	109.5
O2—S1—O1—C8	−154.33 (13)	C13—C8—C9—C10	−1.9 (3)
O3—S1—O1—C8	−24.01 (15)	O1—C8—C9—C10	−178.07 (17)
C1—S1—O1—C8	91.91 (13)	C2—C1—C6—C5	0.4 (3)
O2—S1—C1—C2	−30.49 (18)	S1—C1—C6—C5	−179.20 (14)
O3—S1—C1—C2	−164.75 (15)	C13—O4—C15—C16	−173.64 (17)
O1—S1—C1—C2	79.27 (16)	C13—C12—C11—C10	−1.1 (3)
O2—S1—C1—C6	149.11 (16)	C13—C12—C11—C14	177.62 (18)
O3—S1—C1—C6	14.85 (18)	C6—C1—C2—C3	−0.1 (3)
O1—S1—C1—C6	−101.13 (16)	S1—C1—C2—C3	179.48 (15)
C15—O4—C13—C12	−2.6 (3)	C8—C9—C10—C11	0.1 (3)
C15—O4—C13—C8	176.46 (16)	C12—C11—C10—C9	1.4 (3)
O4—C13—C12—C11	178.42 (16)	C14—C11—C10—C9	−177.30 (19)
C8—C13—C12—C11	−0.6 (3)	C1—C6—C5—C4	−0.1 (3)
O4—C13—C8—C9	−177.01 (16)	C3—C4—C5—C6	−0.4 (3)
C12—C13—C8—C9	2.1 (3)	C7—C4—C5—C6	179.0 (2)

O4—C13—C8—O1	−0.7 (2)	C1—C2—C3—C4	−0.4 (3)
C12—C13—C8—O1	178.41 (15)	C5—C4—C3—C2	0.7 (3)
S1—O1—C8—C9	−87.46 (19)	C7—C4—C3—C2	−178.7 (2)
S1—O1—C8—C13	96.20 (16)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···O3	0.93	2.57	2.926 (2)	103
C2—H2···O1^{i}	0.93	2.58	3.353 (2)	141
C12—H12···O3^{ii}	0.93	2.48	3.310 (2)	149

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1, −*y*, −*z*.

Fig. 1

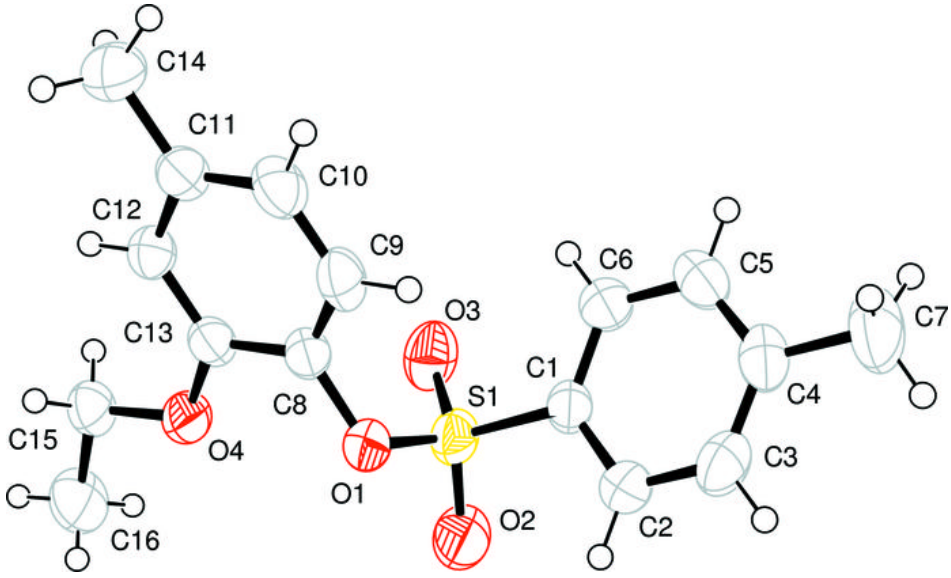

Fig. 2