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Methyl 4-tolyl sulfone

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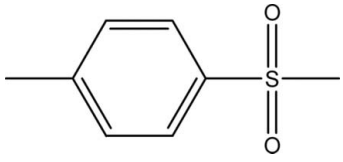
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.109; data-to-parameter ratio = 20.2.

The title compound, $C_8H_{10}O_2S$, was prepared from the reaction of H_2O_2 and methyl 4-tolyl sulfane. The tolyl C atoms are coplanar, the largest deviation being 0.0143 (13) Å for the methyl C atom.

Related literature

For related literature, see: Bahrami (2006); Yang *et al.* (2006).



Experimental

Crystal data

$C_8H_{10}O_2S$
M_r = 170.23
Monoclinic, $P2_1/c$
a = 5.7272 (2) Å
b = 7.9162 (2) Å
c = 18.7857 (5) Å
β = 96.5140 (10)°
V = 846.20 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 298 (2) K
0.25 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.922, T_{max} = 0.937
11134 measured reflections
2041 independent reflections
1773 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
3 standard reflections
frequency: 60 min
intensity decay: 0.3%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.109
S = 1.09
2041 reflections
101 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H9B···O2^{i}	0.96	2.50	3.363 (2)	150
C3—H3···O1^{ii}	0.93	2.59	3.4665 (19)	158

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2165).

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supplementary materials

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Comment

Methyl 4-tolyl sulfone, (I), is an important intermediate in the synthesis of the herbicide Mesotrione (Yang *et al.*, 2006) and was obtained from the reaction of hydrogen peroxide and methyl 4-tolyl sulfane. The molecular structure of (I) is illustrated in Fig. 1. Atoms C1, C2, C3, C4, C5, C6, C7 and S1 are coplanar, the largest deviation being 0.0143 (13) Å for C7. The dihedral angles between the C1—C7/S1 plane and the O1/O2/S1 and C8/01/02 planes are 52.57 (7) and 89.65 (5)^{o}, respectively. C—H···O interactions in the crystal structure of (I) lead to the formation of hydrogen-bonded chains (Table 1 and Fig. 2).

Experimental

The title compound was prepared from hydrogen peroxide and methyl 4-tolyl sulfane, according to the procedure of Bahrami (2006).

Refinement

H atoms were added at calculated positions and refined using a riding model. H atoms were given isotropic displacement parameters equal to 1.2(or 1.5 for methyl H atoms) times the equivalent isotropic displacement parameters of their parent atoms and C—H distances were restrained to 0.93 Å for those bonded to phenyl ring, 0.96 Å for those bonded to methyl.

Figures

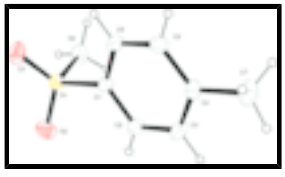

Fig. 1. The structure of (I), shown with 30% probability displacement ellipsoids.

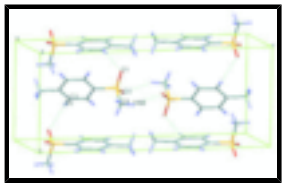

Fig. 2. View showing the C—H···O hydrogen bonding. [Symmetry code: (i) -*x* + 1, -*y* + 2, -*z* (ii) -*x* + 1, +*y* + 1/2, -*z* + 1/2].

Methyl 4-tolyl sulfone

Crystal data

$C_8H_{10}O_2S$ $F_{000} = 360$

M_r = 170.23	D_x = 1.336 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 25 reflections
a = 5.7272 (2) Å	θ = 9.9–13.9º
b = 7.9162 (2) Å	μ = 0.33 mm^{-1}
c = 18.7857 (5) Å	T = 298 (2) K
β = 96.5140 (10)º	Prismatic, colorless
V = 846.20 (4) Å^3	0.25 × 0.20 × 0.20 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.021
Radiation source: fine-focus sealed tube	θ_{max} = 28.2º
Monochromator: graphite	θ_{min} = 2.2º
T = 298(2) K	h = −7→7
ω/2θ scans	k = −10→10
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	l = −25→25
T_{min} = 0.922, T_{max} = 0.937	3 standard reflections
11134 measured reflections	every 60 min
2041 independent reflections	intensity decay: 0.3%
1773 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.1531P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.035	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.109	$\Delta\rho_{max}$ = 0.26 e Å^{-3}
S = 1.09	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
2041 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
101 parameters	Extinction coefficient: 0.009 (3)
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds

in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.2439 (2)	0.81084 (15)	0.06740 (6)	0.0696 (4)
O2	0.6068 (2)	0.9756 (2)	0.09536 (7)	0.0791 (4)
S1	0.35964 (7)	0.95683 (5)	0.099533 (19)	0.05110 (17)
C1	0.3139 (3)	0.96216 (17)	0.19100 (8)	0.0435 (3)
C3	0.4491 (3)	1.0388 (2)	0.31124 (9)	0.0556 (4)
H3	0.5635	1.0873	0.3441	0.067*
C2	0.4838 (3)	1.0346 (2)	0.23968 (9)	0.0525 (4)
H4	0.6195	1.0799	0.2245	0.063*
C4	0.2490 (3)	0.97301 (18)	0.33535 (8)	0.0502 (4)
C5	0.0814 (3)	0.9003 (2)	0.28502 (9)	0.0560 (4)
H7	−0.0544	0.8548	0.3001	0.067*
C6	0.1123 (3)	0.8943 (2)	0.21331 (8)	0.0524 (4)
H8	−0.0011	0.8451	0.1804	0.063*
C8	0.2140 (4)	1.1359 (2)	0.06245 (9)	0.0653 (5)
H9A	0.0484	1.1248	0.0653	0.098*
H9B	0.2416	1.1467	0.0132	0.098*
H9C	0.2720	1.2344	0.0885	0.098*
C7	0.2132 (4)	0.9822 (3)	0.41361 (10)	0.0734 (5)
H10A	0.3471	1.0351	0.4399	0.110*
H10B	0.1949	0.8702	0.4317	0.110*
H10C	0.0748	1.0472	0.4190	0.110*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0963 (10)	0.0634 (7)	0.0455 (6)	0.0132 (6)	−0.0075 (6)	−0.0105 (5)
O2	0.0540 (7)	0.1354 (13)	0.0490 (7)	0.0164 (7)	0.0107 (5)	0.0012 (7)
S1	0.0517 (3)	0.0644 (3)	0.0364 (2)	0.01429 (15)	0.00173 (15)	−0.00173 (14)
C1	0.0433 (7)	0.0488 (7)	0.0374 (7)	0.0055 (5)	0.0004 (5)	−0.0011 (5)
C3	0.0642 (10)	0.0577 (9)	0.0428 (8)	−0.0133 (7)	−0.0026 (7)	−0.0056 (6)
C2	0.0491 (8)	0.0612 (9)	0.0466 (9)	−0.0106 (6)	0.0029 (6)	−0.0016 (6)
C4	0.0619 (9)	0.0470 (7)	0.0417 (8)	0.0026 (6)	0.0067 (7)	0.0011 (6)
C5	0.0465 (8)	0.0677 (9)	0.0544 (9)	−0.0056 (7)	0.0084 (6)	0.0030 (7)
C6	0.0424 (7)	0.0647 (9)	0.0482 (8)	−0.0039 (6)	−0.0031 (6)	−0.0050 (7)
C8	0.0828 (12)	0.0649 (10)	0.0474 (9)	0.0176 (9)	0.0042 (8)	0.0067 (7)
C7	0.0960 (15)	0.0810 (12)	0.0448 (10)	−0.0068 (11)	0.0151 (9)	−0.0005 (8)

Geometric parameters (Å, °)

O1—S1	1.4313 (13)	C4—C7	1.509 (2)
O2—S1	1.4344 (14)	C5—C6	1.379 (2)
S1—C8	1.7487 (17)	C5—H7	0.9300
S1—C1	1.7677 (15)	C6—H8	0.9300
C1—C6	1.381 (2)	C8—H9A	0.9600
C1—C2	1.382 (2)	C8—H9B	0.9600
C3—C4	1.381 (2)	C8—H9C	0.9600
C3—C2	1.381 (2)	C7—H10A	0.9600
C3—H3	0.9300	C7—H10B	0.9600
C2—H4	0.9300	C7—H10C	0.9600
C4—C5	1.393 (2)		
O1—S1—O2	118.25 (9)	C6—C5—C4	121.47 (15)
O1—S1—C8	108.01 (9)	C6—C5—H7	119.3
O2—S1—C8	108.88 (10)	C4—C5—H7	119.3
O1—S1—C1	108.45 (7)	C5—C6—C1	119.16 (14)
O2—S1—C1	107.85 (7)	C5—C6—H8	120.4
C8—S1—C1	104.55 (7)	C1—C6—H8	120.4
C6—C1—C2	120.72 (14)	S1—C8—H9A	109.5
C6—C1—S1	120.45 (11)	S1—C8—H9B	109.5
C2—C1—S1	118.83 (12)	H9A—C8—H9B	109.5
C4—C3—C2	121.76 (14)	S1—C8—H9C	109.5
C4—C3—H3	119.1	H9A—C8—H9C	109.5
C2—C3—H3	119.1	H9B—C8—H9C	109.5
C3—C2—C1	119.06 (15)	C4—C7—H10A	109.5
C3—C2—H4	120.5	C4—C7—H10B	109.5
C1—C2—H4	120.5	H10A—C7—H10B	109.5
C3—C4—C5	117.83 (14)	C4—C7—H10C	109.5
C3—C4—C7	120.72 (16)	H10A—C7—H10C	109.5
C5—C4—C7	121.45 (16)	H10B—C7—H10C	109.5
O1—S1—C1—C6	−29.76 (14)	S1—C1—C2—C3	−179.88 (12)
O2—S1—C1—C6	−158.93 (13)	C2—C3—C4—C5	0.4 (2)
C8—S1—C1—C6	85.30 (14)	C2—C3—C4—C7	−178.81 (16)
O1—S1—C1—C2	149.93 (12)	C3—C4—C5—C6	−0.2 (2)
O2—S1—C1—C2	20.76 (15)	C7—C4—C5—C6	178.95 (16)
C8—S1—C1—C2	−95.02 (14)	C4—C5—C6—C1	−0.1 (2)
C4—C3—C2—C1	−0.2 (2)	C2—C1—C6—C5	0.3 (2)
C6—C1—C2—C3	−0.2 (2)	S1—C1—C6—C5	−179.98 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H9B···O2^{i}	0.96	2.50	3.363 (2)	150
C3—H3···O1^{ii}	0.93	2.59	3.4665 (19)	158

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*; (ii) −*x*+1, *y*+1/2, −*z*+1/2.

Fig. 1

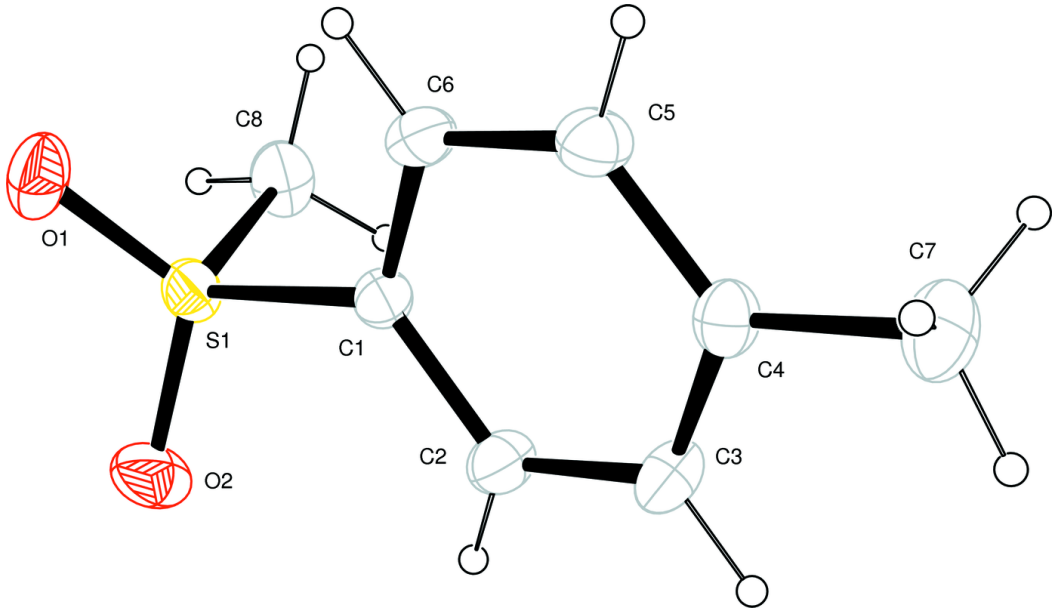

Fig. 2