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1-Phenyl-2-(toluene-4-sulfonyl)ethanone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.104
Data-to-parameter ratio = 10.1

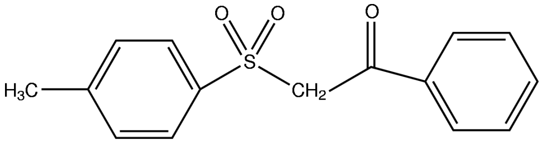
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $C_{15}H_{14}O_3S$, displays a stair-like arrangement, with the tolyl and phenyl rings forming the steps. The S atom lies in the plane of the tolyl ring, whereas the ketone group $CO(CH_2)$ is coplanar with the phenyl ring.

Comment

β-Keto sulfones have attracted considerable interest, because they are versatile intermediates for the synthesis of complex natural products and biologically active compounds (Simpkins, 1993; Fuchs & Braisch, 1986).

As shown in Fig. 1, the title compound, (I), displays a stair-like arrangement. The two steps contain the tolyl and phenyl rings linked by the SO_2CH_2CO group. Atoms C2, O1 and C1 of the ketone group $CO(CH_2)$ are nearly coplanar with the phenyl ring; indeed, these atoms deviate from the mean plane of the phenyl ring by 0.009, −0.06 and 0.153 Å, respectively. This planarity is certainly the result of *π*-system conjugation. The S atom of the sulfoxide group is coplanar with the tolyl ring (deviation from the tolyl plane 0.008 Å).



(I)

The two mean planes forming the steps are nearly parallel to each other, with a dihedral angle between them of 3.3°. The distance of 1.86 Å between these two planes is close to the value of 1.783 (2) Å observed for the C1—S1 bond.

The packing of molecules in the unit cell is governed by weak C—H···O interactions, as shown in Fig. 2.

Experimental

Sodium *p*-toluenesulfinate (3.72 g, 21 mmol) in 1,2-dimethoxyethane (25 ml) was added to a solution of 2-bromo-1-phenylethanone

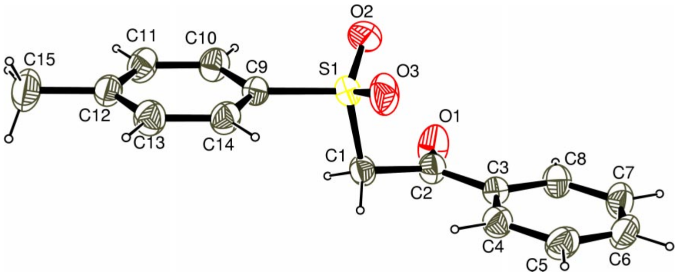


Figure 1
A view of the molecular structure of (I), with 30% probability displacement ellipsoids.

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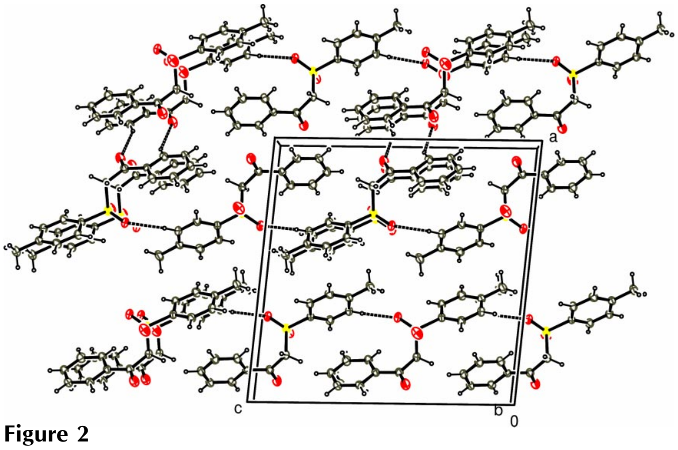

Figure 2
The crystal packing of (I), showing the weak C—H···O interactions as dashed lines. Displacement ellipsoids are drawn at the 20% probability level.

(3.96 g, 20 mmol) and tetrabutylammonium bromide (0.33 g, 1.0 mmol). The mixture was heated under reflux for 30 min. After cooling, iced water was added and the white precipitate which formed was collected, washed with water and recrystallized from ethanol (Wildeman & Leusen, 1979) to obtain single crystals of (I) suitable for X-ray analysis.

Crystal data

$C_{15}H_{14}O_3S$
$M_r = 274.33$
Monoclinic, $P2_1/c$
$a = 15.8077$ (7) Å
$b = 5.4113$ (2) Å
$c = 15.8940$ (9) Å
$\beta = 95.343$ (2)°
$V = 1353.7$ (1) Å^3
$Z = 4$
$D_x = 1.346$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9916 reflections
$\theta = 1.7$–27.3°
$\mu = 0.24$ mm^{-1}
$T = 293.1$ K
Chunk, colourless
0.40 × 0.24 × 0.14 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.862$, $T_{\max} = 0.967$
10 775 measured reflections
2861 independent reflections
1729 reflections with $F^2 > 2\sigma(F^2)$
$R_{\rm int} = 0.035$
$\theta_{\max} = 27.3°$
$h = -20 \rightarrow 20$
$k = -6 \rightarrow 6$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.104$
$S = 1.01$
1729 reflections [but 1729 above?]
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0644P)^2 + 0.233P]$ where $P = 0.333\max(F_o^2,0) + 0.667F_c^2$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.17$ e Å^{-3}
$\Delta\rho_{\min} = -0.26$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.428 (2)	O1—C2	1.210 (3)
S1—O3	1.433 (2)	C1—C2	1.520 (3)
S1—C1	1.782 (3)	C2—C3	1.483 (4)
S1—C9	1.756 (3)		
O2—S1—O3	118.87 (14)	S1—C1—C2	109.94 (18)
O2—S1—C1	107.26 (13)	C1—C2—O1	117.5 (2)
O3—S1—C1	108.37 (13)	C1—C2—C3	120.5 (2)
O2—S1—C9	108.90 (13)	O1—C2—C3	122.0 (2)
O3—S1—C9	108.75 (13)	C2—C3—C4	123.2 (2)
C1—S1—C9	103.63 (12)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···O1$^{\rm i}$	0.93	2.52	3.341 (3)	147
C11—H11···O3$^{\rm ii}$	0.93	2.46	3.388 (3)	171

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $x, \frac{3}{2}-y, z-\frac{1}{2}$.

The H atoms were placed in calculated positions, with C—H = 0.96–0.98 Å, and were included in the final cycles of the refinement in a riding model, with $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}$ of the carrier atoms.

Data collection: *PROCESS-AUTO* (Rigaku, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku, 2004); program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Watkin *et al.*, 1996); molecular graphics: *ORTEP*-3 *for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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