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1-Napthyl 4-toluenesulfonate: supramolecular aggregation through weak C—H···O and C—H···π interactions

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.036
wR factor = 0.092
Data-to-parameter ratio = 17.0

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

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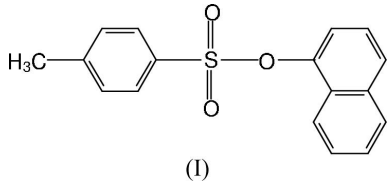
In the crystal structure of the title compound, $C_{17}H_{14}O_3S$, the dihedral angle between the mean planes of the 4-tolyl and 1-naphthyl rings is 45.05 (4)°. The supramolecular aggregation is completed by the presence of intermolecular C—H···O and C—H···π interactions.

Comment

Aromatic sulfonates have biological importance (Yachi *et al.*, 1989; Spungin *et al.*, 1992; Tharakan *et al.*, 1992; Alford *et al.*, 1991; Jiang *et al.*, 1990; Narayanan & Krakow, 1983). The crystal structure of the title compound, (I), was determined for this reason.



(I)

The S—C, S—O and S═O bond lengths (Table 1) are comparable with those found in related structures (Vembu, Nallu, Garrison & Youngs, 2003*a*,*b*,*c*,*d*,*e*,*f*; Vembu, Nallu, Spencer & Howard, 2003*a*,*b*,*c*,*d*,*e*,*f*,*g*; Vembu *et al.*, 2003; Vembu, Nallu, Durmus *et al.*, 2004*a*,*b*,*c*).

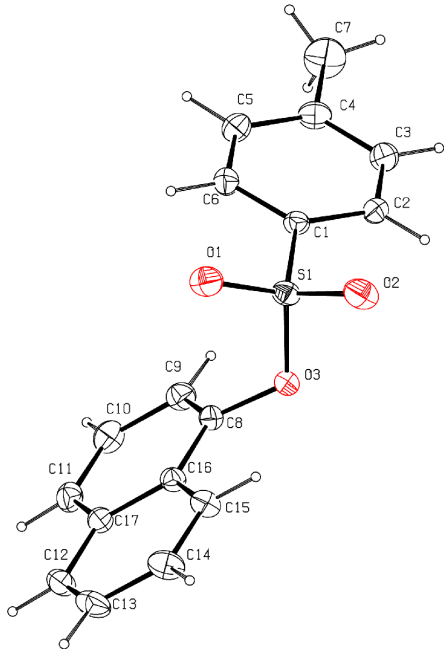


Figure 1
The molecular structure of the title compound, showing 50% probability ellipsoids.

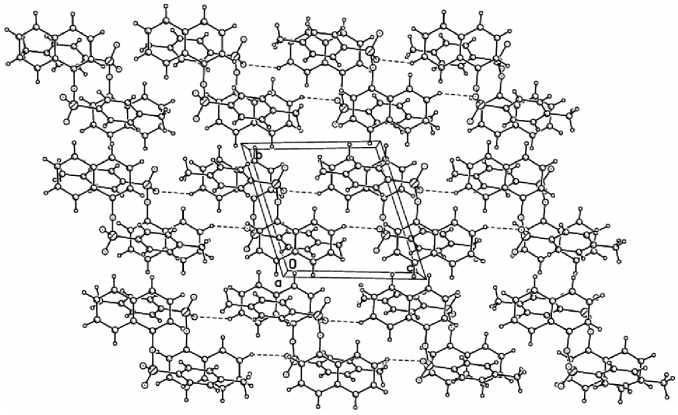


Figure 2
Packing of the the title compound, viewed down the *a* axis

The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. The dihedral angle between the mean planes of the 4-tolyl and 1-naphthyl rings is 45.05 (4)°. This contrasts with the near coplanar orientation observed in 2,4-dinitrophenyl 4-toluenesulfonate (Vembu, Nallu, Garrison & Youngs, 2003*a*), 4-methoxyphenyl 4-toluenesulfonate (Vembu *et al.*, 2003) and 8-quinolyl 3-nitrobenzenesulfonate (Vembu, Nallu, Spencer & Howard, 2003*e*).

The crystal structure of (I) is stabilized by weak C—H···O (Fig. 2 and Table 2) and C—H···π interactions. The range for the H···O distances found in (I) agrees with those found for weak C—H···O bonds (Desiraju & Steiner, 1999).

Experimental

4-Toluenesulfonyl chloride (4.7 mmol), dissolved in acetone (4 ml) was added dropwise to 1-naphthol (4.2 mmol) in aqueous NaOH (2.5 ml, 10%) with constant shaking. The precipitated title compound (3.2 mmol, yield 76%) was filtered off and recrystallized from aqueous ethanol.

Crystal data

$C_{17}H_{14}O_3S$
M_r = 298.34
Triclinic, $P\overline{1}$
a = 8.8693 (10) Å
b = 9.3982 (10) Å
c = 9.7112 (10) Å
α = 70.446 (4)°
β = 71.335 (4)°
γ = 81.831 (8)°
V = 722.12 (14) Å^3
Z = 2
D_x = 1.372 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3629 reflections
θ = 2.5–30.0°
μ = 0.23 mm^{-1}
T = 120 K
Fragment, tan
0.40 × 0.27 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer with an Oxford Cryosystems Cryostream cooler
ω scans with κ offsets
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
T_{min} = 0.934, T_{max} = 0.982
12 785 measured reflections
4173 independent reflections
3618 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 30.1°
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.092
S = 1.05
4173 reflections
246 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0371P)^2 + 0.2951P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O2	1.4244 (9)	S1—C1	1.7513 (11)
S1—O1	1.4296 (9)	O3—C8	1.4105 (14)
S1—O3	1.6068 (9)		
O2—S1—O1	120.59 (6)	O1—S1—C1	109.43 (6)
O2—S1—O3	103.28 (5)	O3—S1—C1	103.66 (5)
O1—S1—O3	108.74 (5)	C8—O3—S1	119.57 (7)
O2—S1—C1	109.69 (6)		
O2—S1—O3—C8	158.11 (8)	C1—S1—O3—C8	−87.46 (9)
O1—S1—O3—C8	28.90 (10)		

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of rings C1–C6, C8–C11/C16/C17 and C12–17, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O2^{i}	0.968 (17)	2.975 (17)	3.7990 (16)	143.8 (12)
C6—H6···O1^{ii}	0.986 (16)	2.621 (16)	3.4334 (15)	139.8 (12)
C7—H7*A*···O2^{iii}	0.96 (3)	2.69 (3)	3.515 (2)	144.1 (18)
C14—H14···O1^{iv}	0.976 (18)	2.509 (18)	3.3231 (16)	140.8 (14)
C2—H2···*Cg*2^{v}	0.973 (16)	2.68	3.36	127
C3—H3···*Cg*3^{v}	0.968 (17)	2.83	3.40	119
C5—H5···*Cg*3^{vi}	0.998 (17)	2.86	3.55	127
C6—H6···*Cg*2^{vi}	0.986 (16)	3.01	3.62	121
C11—H11···*Cg*1^{vii}	0.960 (17)	2.78	3.49	132

Symmetry codes: (i) $-x, 2-y, 2-z$; (ii) $1-x, 1-y, 2-z$; (iii) $x, y, 1+z$; (iv) $1-x, 1-y, 1-z$; (v) $-x, 1-y, -z$; (vi) $1-x, 1-y, -z$; (vii) $x, y-1, z$.

All H atoms were located in a difference Fourier map and their positions and displacement parameters were refined.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; 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*.

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