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8-(Tolyl-4-sulfonyloxy)quinolinium toluene-4-sulfonate

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Key indicators

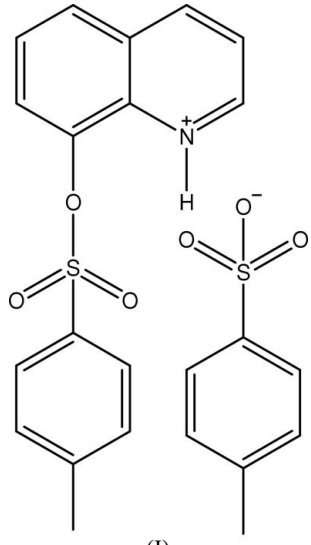
Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.004 Å
R factor = 0.042
wR factor = 0.120
Data-to-parameter ratio = 14.1

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

In the cation of the title compound, $C_{16}H_{14}NO_3S^+\cdot C_7H_7O_3S^-$, the quinolinium ring system makes a dihedral angle of 69.14 (9)° with the benzene ring.

Comment

Derivatives of 8-hydroxyquinoline are known for their anti-amoebic, antibacterial and antifungal activities (Balasubramanian & Thomas Muthiah, 1996; Khan *et al.*, 1994; Vembu *et al.*, 2003). The title compound, (I), is an intermediate in the synthesis of 8-hydroxyquinoline derivatives (Lee *et al.*, 2001). We report here the crystal structure of (I) (Fig. 1).



(I)

The benzene C10–C15 and C22–C17 planes make dihedral angles of 69.14 (9) and 78.31 (6)°, respectively, with the C1–C9/N1 plane. The dihedral angle between the two benzene rings is 61.74 (9)°.

In the crystal structure of (I), there are C—H···O and N—H···O hydrogen bonds (Table 1).

Experimental

A solution of 8-hydroxyquinoline (6.9 mmol) in dichloromethane (6 ml) was added dropwise to 4-toluenesulfonyl chloride (20.5 mmol) and the mixture was refluxed in air for 4 h. The resultant precipitate was filtered off and the solution was evaporated to give (I) as a deep-yellow solid. Single crystals suitable for X-ray diffraction were obtained by recrystallization from an acetone solution.

Crystal data

$C_{16}H_{14}NO_3S^+\cdot C_7H_7O_3S^-$
M_r = 471.53
Triclinic, $P\overline{1}$
a = 9.643 (5) Å
b = 10.852 (5) Å
c = 11.421 (5) Å
α = 105.470 (5)°
β = 97.976 (5)°
γ = 99.295 (5)°
V = 1115.8 (9) Å^3
Z = 2
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 292 (2) K
Block, yellow
0.45 × 0.26 × 0.24 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.886, T_{max} = 0.936
8405 measured reflections
4111 independent reflections
3208 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.120
S = 1.03
4111 reflections
291 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0577P)^2 + 0.4629P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O4^{i}	0.86	1.89	2.703 (3)	158
C4—H4···O3^{ii}	0.93	2.33	3.256 (3)	173
C8—H8···O5^{i}	0.93	2.54	3.358 (4)	146
C15—H15···O4^{i}	0.93	2.49	3.162 (3)	130
C18—H18···O5^{i}	0.93	2.59	3.288 (3)	132

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

H atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; 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*.

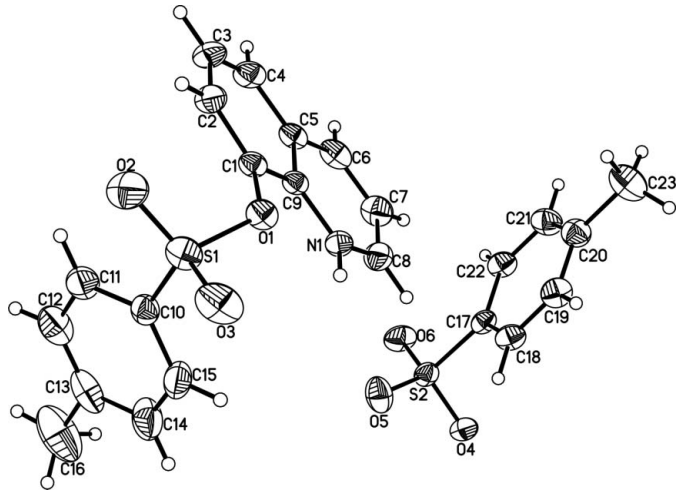


Figure 1
The molecular structure of (I), showing 30% probability displacement ellipsoids and the atomic numbering.

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