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5,7-Dibromo-*N*-tosylquinolin-8-amine

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.007 Å
R factor = 0.041
wR factor = 0.109
Data-to-parameter ratio = 14.3

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

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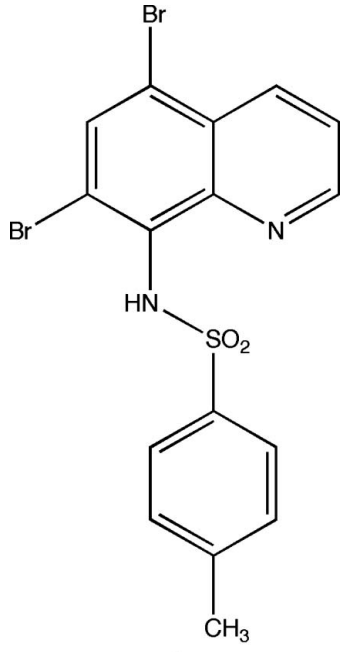
In the crystal structure of the title compound, $C_{16}H_{12}Br_2N_2O_2S$, molecules are linked by two hydrogen bonds to form a three-dimensional network. The H atom of the NH group has two intermolecular contacts; one to a sulfonyl O atom (H···O = 2.22 Å) and the other to the Br at the quinoline C-7 position (H···Br = 3.11 Å).

Comment

The investigation of the crystal structure of the title compound, (I), is part of our search for Zinquin Ester analogues (Kimber *et al.*, 2000). This class of compounds has been shown to be effective in the detection of zinc (II) in a range of mammalian cells (Pearce *et al.*, 2001).



(I)

The molecular structure of the title compound (I) is illustrated in Fig. 1. The quinoline ring system is planar and inclined to the benzene ring of the tosyl moiety [torsion angle C1—N1—S1—C10 being 76.5 (3)°].

The crystal packing of (I) is stabilized through a hydrogen-bonding network, as shown in Fig. 2. Details of the hydrogen bonding are given in Table 1.

Experimental

Compound (I) was prepared according to the literature procedure (Xue *et al.*, 2000). Suitable crystals were obtained by recrystallization from methanol-dichloromethane (1:1).

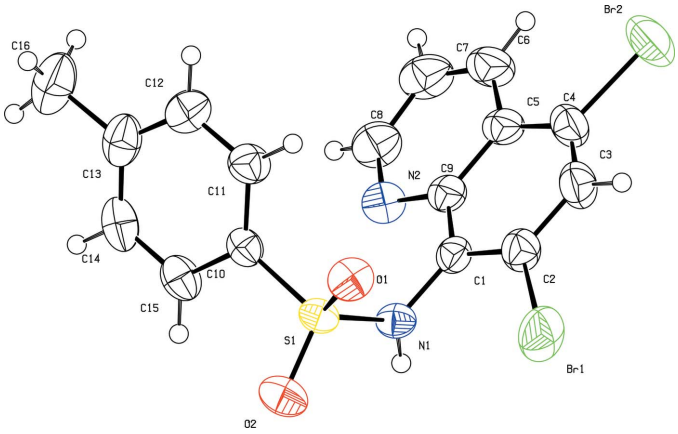


Figure 1
Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

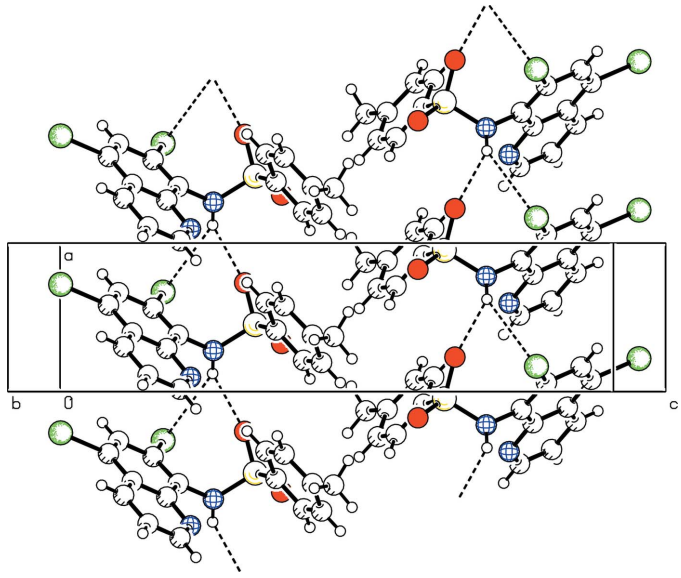


Figure 2
The packing of (I), with hydrogen bonding shown as dashed lines.

Crystal data

$C_{16}H_{12}Br_2N_2O_2S$
M_r = 456.16
Orthorhombic, $P2_12_12_1$
a = 4.939 (1) Å
b = 16.595 (3) Å
c = 20.254 (4) Å
V = 1660.1 (6) Å^3
Z = 4
D_x = 1.825 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 5.3–18.8°
μ = 7.46 mm^{-1}
T = 299 (2) K
Long needle, light brown
0.65 × 0.08 × 0.05 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.486, T_{max} = 0.708
3465 measured reflections
2997 independent reflections
2758 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 68.0°
$h = 0 \rightarrow 5$
$k = 0 \rightarrow 19$
$l = -24 \rightarrow 24$
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.109
S = 1.08
2997 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.076P)^2 + 0.4357P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.92 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0012 (2)
Absolute structure: Flack (1983)
Flack parameter: −0.01 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···O1^{i}	0.86	2.22	2.884 (4)	134
N1—H1*N*···Br1^{i}	0.86	3.11	3.873 (3)	149

Symmetry code: (i) $x-1, y, z$.

The H atoms were included in idealized positions and refined as riding atoms with U_{iso}(H) = 1.2U_{eq}(parent atom), and N—H = 0.86 Å and C—H = 0.93 Å (0.96 Å for methyl groups).

Data collection: *Nonius Diffractometer Control Software* (Nonius, 1996); cell refinement: *Nonius Diffractometer Control Software*; data reduction: *REDU4* (Stoe & Cie, 1987); 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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