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Quinolin-8-yl 2,5-dichlorobenzenesulfonate

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.132
Data-to-parameter ratio = 13.0

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

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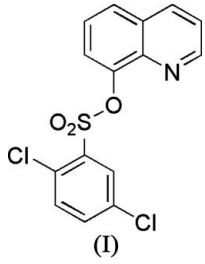
In the title compound, $C_{15}H_9Cl_2NO_3S$, the torsion angle about the O—S bond between the quinoline system and the benzene ring is 146.2 (2)°. One weak intermolecular C—H···O hydrogen bond is observed in the crystal structure.

Comment

Quinoline derivatives have been reported to show broad-spectrum efficacy against multiple herpes viruses and they may have a potential role for the treatment of a variety of infections, such as those caused by herpes simplex virus type 1 (Hartline *et al.*, 2005; Oliveira *et al.*, 2004), human cytomegalovirus and varicella zoster virus (Oien *et al.*, 2002; Knechtel *et al.*, 2002). As part of our screening programme to investigate antiviral activity (Andrighetti-Fröhner *et al.*, 2003; Savi *et al.*, 2005), we report here an X-ray crystallographic study of the title compound, (I).



(I)

The key feature of the molecular structure of (I) (Fig. 1) is the C1—O1—S1—C10 torsion angle of 146.2 (2)°, which illustrates the non-planarity of the molecule. The H atom on atom C3 of the quinoline ring system has one intermolecular contact to a sulfonyl O atom (H···O = 2.54 Å), forming a three-dimensional network (Fig. 2 and Table 1).

Experimental

The title compound was prepared by the reaction of one equivalent of 8-hydroxyquinoline and 1.1 equivalents of 2,5-dichlorobenzenesulfonyl chloride in the presence of pyridine (2 ml) overnight, according to the literature procedure of Kimber *et al.* (2003). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from a solution in methanol–dichloromethane (1:1).

Crystal data

$C_{15}H_9Cl_2NO_3S$
M_r = 354.19
Monoclinic, $P2_1/c$
a = 7.842 (1) Å
b = 25.536 (3) Å
c = 7.642 (1) Å
β = 107.87 (1)°
V = 1456.5 (3) Å^3
Z = 4
D_x = 1.615 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 5.46 mm^{-1}
T = 299 (2) K
Prism, colourless
0.53 × 0.30 × 0.23 mm

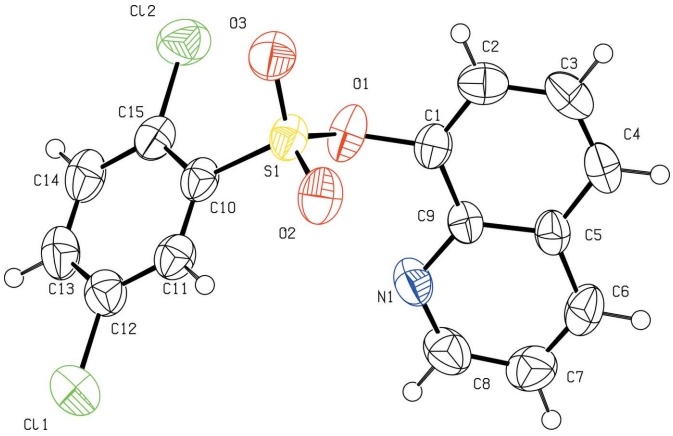


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

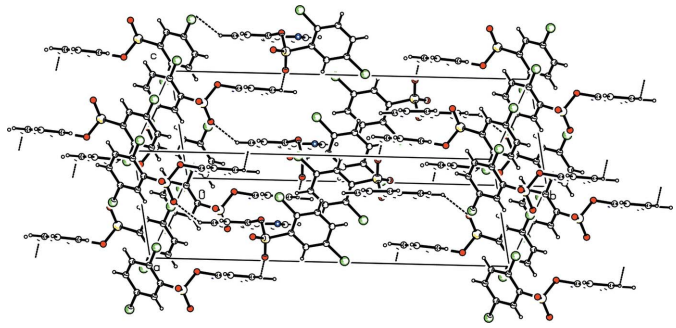


Figure 2
The packing of (I), showing the hydrogen bonding (dashed lines).

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.129, T_{max} = 0.285
3088 measured reflections
2593 independent reflections
2301 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 67.0°
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.132
S = 1.07
2593 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2 + 0.9445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0045 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O2^{i}	0.93	2.54	3.294 (4)	138

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

All H atoms were positioned with idealized geometry, with C—H = 0.93 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD-4-PC* (Enraf–Nonius, 1993); cell refinement: *CAD-4-PC*; 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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