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2-Aminoquinolin-8-yl 4-fluorobenzenesulfonate

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.125
Data-to-parameter ratio = 10.6

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

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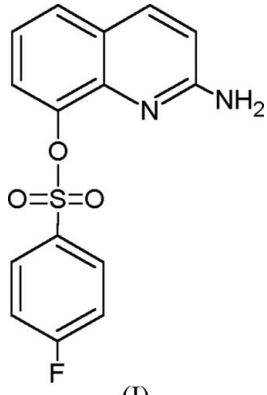
The molecular packing of the title compound, $C_{15}H_{11}N_2O_3S$, is stabilized by a hydrogen-bonded network. The H atoms of the amino group form intermolecular N—H···N [2.13 (3) Å] and N—H···O [2.46 (3) Å] hydrogen bonds. The sulfonyl O atoms are each also involved in intermolecular C—H···O hydrogen bonds [H···O = 2.56 (3) and 2.45 (3) Å].

Comment

Arylsulfonyl substituents have been used as protecting groups for oxygen and nitrogen functionalities (O'Connell & Rapoport, 1992). Furthermore, 2-aminoquinoline derivatives have been prepared and assayed as melanin- concentrating hormone (MCH)1*R* antagonists (Jiang *et al.*, 2006). In addition, 2-aminoquinoline has shown antibacterial and anthelmintic activities (Pfister, 1988). We sought to synthesize heterocycle compounds and evaluate their antiparasitic activity (Jain *et al.*, 2005). In this context, the title compound, (I), was obtained and we report here the crystal stucture analysis.



(I)

In the molecule of (I) (Fig. 1), the quinoline ring system, with the amino group, is nearly planar with maximum deviations from the mean plane of −0.026 (2) Å for atom C7 and 0.024 (2) Å for atom C4. The torsion angle about the central bridge (C1—O3—S1—C10) is 77.9 (2)° and the aminoquinoline plane forms a dihedral angle of 49.78 (2)° with the plane of the aromatic ring of the toluenesulfonate group. The molecular packing of (I) is stabilized by hydrogen bonds (details are given in Table 1).

Experimental

Compound (I) was prepared by the overnight reaction of 50 mg (0.31 mmol) of 2-amino-8-hydroxyquinoline and 66.8 mg (0.34 mmol)

of fluorobenzenesulfonyl chloride in the presence of 2 ml of pyridine at 273 K with stirring. The resulting mixture was poured on to ice, filtered and washed with water. Single crystals suitable for X-ray data collection were obtained by recrystallization of the crude product (75 mg) from a methanol–dichloromethane (1:1) solution of (I), yielding a light brown crystalline solid (75%), m.p. 469 K.

Crystal data

$C_{15}H_{11}FN_2O_3S$
M_r = 318.32
Triclinic, $P\overline{1}$
a = 7.8513 (9) Å
b = 8.0764 (9) Å
c = 11.680 (1) Å
α = 89.482 (9)°
β = 79.070 (9)°
γ = 77.738 (9)°
V = 710.23 (13) Å^3
Z = 2
D_x = 1.488 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.28 mm^{-1}
T = 299 (2) K
Plate, light brown
0.40 × 0.23 × 0.05 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.382, T_{max} = 0.792
(expected range = 0.430–0.892)
3581 measured reflections
2470 independent reflections
2023 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 66.9°
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.125
S = 1.03
2470 reflections
232 parameters
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.079P)^2 + 0.1361P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.010
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21*N*···N1^{i}	0.90 (3)	2.13 (3)	3.007 (3)	167 (3)
N2—H22*N*···O1^{i}	0.85 (3)	2.46 (3)	3.150 (3)	140 (3)
C6—H6···O1^{ii}	0.97 (3)	2.56 (3)	3.517 (3)	167 (2)
C12—H12···O2^{iii}	0.89 (3)	2.45 (3)	3.317 (4)	166 (3)

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

The H atoms were located in a difference map and their positional parameters were refined. Their isotropic displacement parameters were set to $1.2U_{eq}$ of the parent atom.

Data collection: *CAD-4-PC* Software (Nonius, 1996); cell refinement: *CAD-4-PC* Software; data reduction: *REDU4* (Stoe, 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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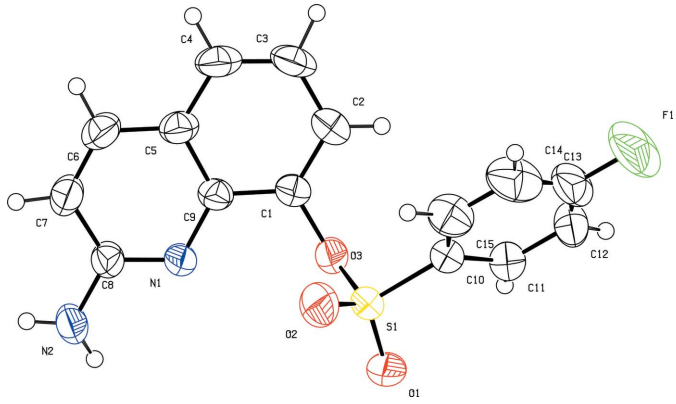

Figure 1
The molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius.

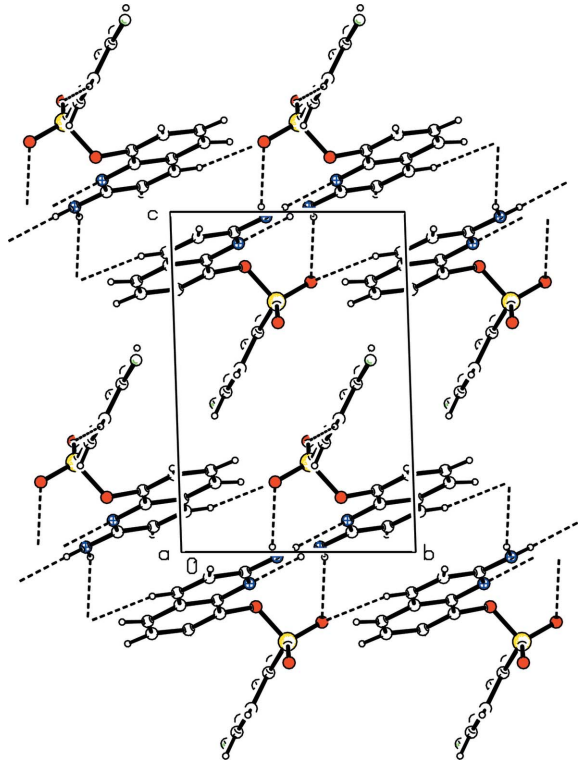

Figure 2
Molecular packing of (I) with hydrogen bonds shown as dashed lines.

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