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2-Aminoquinolin-4-yl 2,4,6-triisopropylbenzenesulfonate

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.006 Å
Disorder in main residue
R factor = 0.057
wR factor = 0.152
Data-to-parameter ratio = 13.9

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

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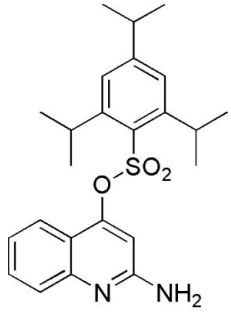
The molecular packing of the title compound, $C_{24}H_{30}N_2O_3S$, is stabilized by a hydrogen-bonded network. Both sulfonyl O atoms are involved in intermolecular hydrogen bonds of types N—H···O and C—H···O. An intermolecular N—H···N hydrogen bond is also observed.

Comment

Quinolines comprise an important class of heterocyclic compounds present in many potent biologically active molecules (Frank *et al.*, 2004). In addition, aminoquinoline derivatives have shown cytotoxic activity (Kim *et al.*, 2005), as well as antibacterial, antifungal and antiparasitic activities (Jain *et al.*, 2005). A large number of quinoline derivatives have been synthesized because the quinoline unit has well defined and attractive ionophoric properties toward a variety of important metal ions (Yoshida *et al.*, 2002). The specific properties of the quinoline fluorophores that exhibit dramatic fluorescence enhancement upon complexation with guest molecules will be useful for fundamental research into solid-state fluorescence and for the development of new intense solid-emissive materials (Ooyama *et al.*, 2005). Our interest in such metal chelators is as potential agents for neuroprotection in neurodegenerative diseases (Zheng *et al.*, 2005); in connection with this research, we describe in this paper the crystallographic study of the title compound, (I).



(I)

The quinoline ring system, with the amino group, is nearly planar, with maximum deviations from the mean plane of −0.032 (3) Å for atom N1 and 0.042 (3) Å for atom N2. The quinoline unit forms a C1—O1—S1—C10 torsion angle with the benzene ring of 87.7 (2)°. Three intermolecular hydrogen bonds of types N—H···O, N—H···N and C—H···O are observed; these connect molecules to form a three-dimensional network (Fig. 2). Details of the hydrogen-bonding parameters are given in Table 1.

Experimental

Compound (I) was prepared according to a literature procedure (Xue *et al.*, 2000). Crystals suitable for X-ray diffraction analysis were obtained by recrystallization from a methanol–dichloromethane solution (1:1).

Crystal data

$C_{24}H_{30}N_2O_3S$
M_r = 426.56
Triclinic, $P\overline{1}$
a = 9.431 (1) Å
b = 11.015 (2) Å
c = 12.312 (2) Å
α = 77.61 (1)°
β = 80.79 (1)°
γ = 69.11 (1)°
V = 1162.2 (3) Å^3
Z = 2
D_x = 1.219 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 299 (2) K
Prism, yellow
0.28 × 0.13 × 0.08 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
4540 measured reflections
3997 independent reflections
2461 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 66.9°
3 standard reflections
frequency: 120 min
intensity decay: 2.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.152
S = 1.02
3997 reflections
287 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0729P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.012
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21*N*···O3^{i}	0.84 (4)	2.37 (4)	3.197 (4)	167 (4)
N2—H22*N*···N1^{ii}	0.85 (4)	2.22 (4)	3.073 (4)	175 (4)
C9—H9···O2^{i}	0.93	2.60	3.522 (4)	174

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

The amino H atoms were located in a difference map and refined freely. Carbon-bound H atoms were positioned with idealized geometry using a riding model (C—H = 0.93–0.98 Å). All H atoms were refined with isotropic displacement parameters (set at 1.2 times of the U_{eq} of the parent atom). Atom C20 of the methyl group is disordered and was refined with a split model. The corresponding site-occupation factors were refined, but were later fixed at 0.65:0.35.

Data collection: *CAD-4-PC* (Nonius, 1996); 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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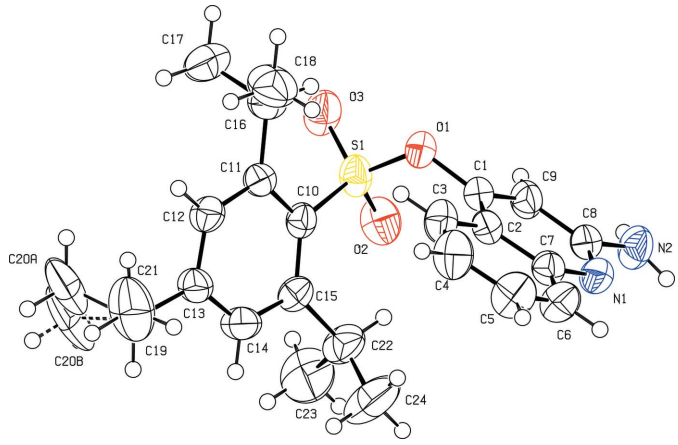

Figure 1
The molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. The minor disorder components are shown with dashed bonds.

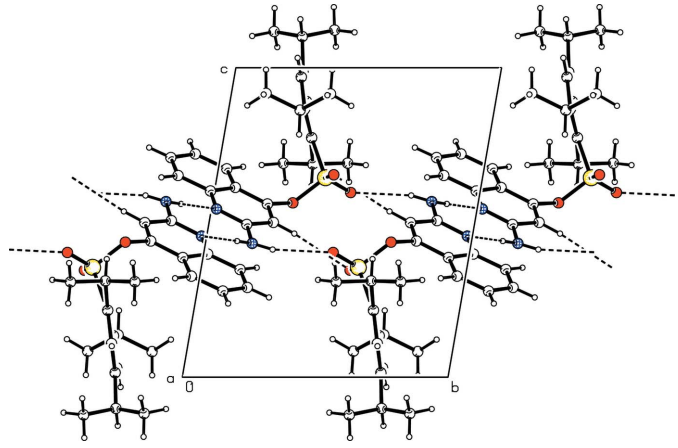

Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines.

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