Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Aminoquinolin-8-yl 2,4,6-triisopropylbenzenesulfonate

Luiz Everson da Silva,[a] Sabine Foro[b] and Boris Schmidt[b]*

[a]Universidale Federal de Mato Grosso, Departamento de Química–UFMT, 78060-900 Cuiabá, MT, Brazil, and [b]Clemens Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany

Correspondence e-mail: foro@tu-darmstadt.de

Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.007 Å
R factor = 0.058
wR factor = 0.182
Data-to-parameter ratio = 15.6

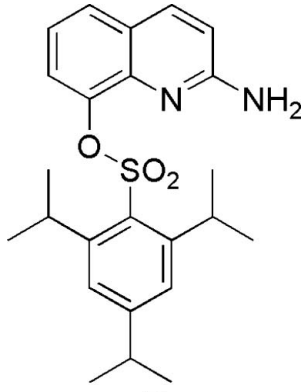
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 December 2006
Accepted 13 December 2006

The nearly planar aminoquinoline fragment and the aromatic ring of the triisopropylbenzenesulfonate group of the title compound, $C_{24}H_{30}N_2O_3S$, form a dihedral angle of 47.9 (2)°. Both H atoms of the amino group are involved in intermolecular hydrogen bonds of types N—H···O (2.56 Å) and N—H···N (2.26 Å), linking the molecules into dimers.

Comment

Aminoquinoline derivatives are precursors to a number of antiparasitic drugs (O'Neill *et al.*, 1998). Moreover, many antimalarial compounds which incorporate the quinoline ring system have shown antiprion activity (Kocisko & Caughey, 2006). In addition, the 8-hydroxyquinoline (8-HQ) system has received continuing attention as a platform for the construction of a number of selective and efficient ionophores (Youk *et al.*, 2004). These organic fluorophores have received much attention in recent years, because of their many applications in the optoelectronics industry, as well as in the treatment of neurodegenerative diseases (Ooyama *et al.*, 2005; Raman *et al.*, 2005). Our interest in metal chelators based on this quinoline core, as potential agents for neuroprotection in Alzheimer's disease (Zheng *et al.*, 2005), led to the X-ray crystallographic study of the title compound, (I).



(I)

The quinoline ring system of (I), with the amino group, is nearly planar, with maximum deviations from the mean plane of −0.041 (3) Å for atom C9 and 0.048 (2) Å for atom N2. The quinoline unit forms a C1—O3—S1—C10 torsion angle with the benzene ring of 88.5 (2)°.

Two intermolecular hydrogen bonds of types N—H···O and N—H···N are observed, and these link the molecules in the structure into dimeric aggregates (Fig. 2). Details of the hydrogen-bonding parameters are given Table 1.

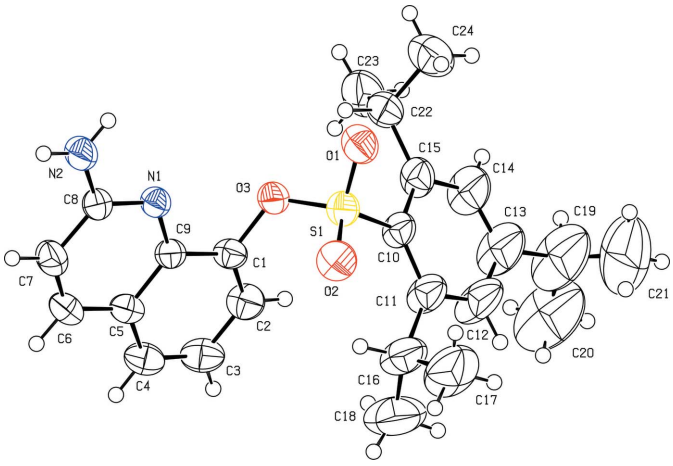


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

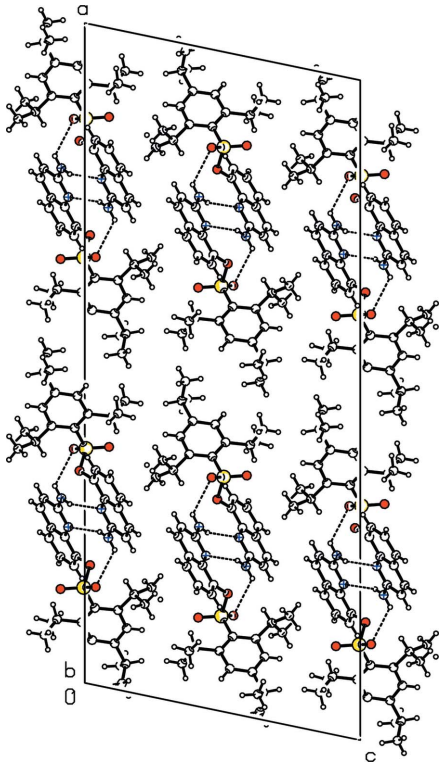


Figure 2
The molecular packing of (I), with hydrogen bonds shown as dashed lines.

Experimental

2-Amino-8-hydroxyquinoline (50 mg, 0.31 mmol) and 2,4,6-triisopropylbenzenesulfonyl chloride (103 mg, 0.34 mmol) were dissolved in pyridine (2 ml) at 273 K with stirring and left to stand overnight. 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 (105 mg) from a methanol–dichloromethane (1:1) solution of (I). The product was a colourless solid (yield 72%; m.p. 446 K).

Crystal data

$C_{24}H_{30}N_2O_3S$
M_r = 426.56
Monoclinic, $C2/c$
a = 40.435 (3) Å
b = 7.0362 (4) Å
c = 17.212 (2) Å
β = 101.754 (9)°
V = 4794.3 (7) Å^3
Z = 8
D_x = 1.182 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 299 (2) K
Prism, light brown
0.28 × 0.10 × 0.06 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
4693 measured reflections
4286 independent reflections
2749 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 67.0°
3 standard reflections
frequency: 120 min
intensity decay: 2.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.182
S = 1.06
4286 reflections
275 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0995P)^2 + 1.8788P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.44 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—H22N···O1^{i}	0.86	2.56	3.137 (4)	125
N2—H21N···N1^{i}	0.86	2.26	3.066 (4)	156

Symmetry code: (i) $-x+\frac{1}{2}, -y+\frac{5}{2}, -z$.

The H atoms were positioned with idealized geometry and refined using a riding model, with C—H = 0.93–0.98 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N) or 1.5U_{eq}(methyl C). Atoms C20 and C21 of one of the isopropyl groups display elongated ellipsoids, suggesting the presence of disorder. However, no reliable disorder model could be produced. The U^{ij} components of these atoms were restrained to approximate isotropic behaviour, and the C—C lengths were restrained to 1.530 (7) Å.

Data collection: *CAD-4-PC Software* (Nonius, 1996); cell refinement: *CAD-4-PC 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*.

The authors thank Professor Dr Hartmut Fuess, Technische Universität Darmstadt, for diffractometer time.

References

Kocisko, D. A. & Caughey, B. (2006). *J. Virol.* **80**, 1044–1046.
Nonius (1996). *CAD-4-PC Software*. Version 2.0. Nonius GmbH, Solingen, Germany.
O'Neill, P. M., Bray, P. G., Hawley, S. R., Ward, S. A. & Park, B. K. (1998). *Pharmacol. Ther.* **77**, 29–58.
Ooyama, Y., Nakamura, T. & Yoshida, K. (2005). *New J. Chem.* **29**, 447–456.
Raman, B., Ban, T., Yamaguchi, K., Sakai, M., Kawai, T., Naiki, H. & Goto, Y. (2005). *J. Biol. Chem.* **280**, 16157–16162.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.
Youk, J.-S., Kim, Y. H., Kim, E.-J., Youn, N. J. & Chang, S.-K. (2004). *Bull. Korean Chem. Soc.* **25**, 869–872.
Zheng, H., Weiner, L. M., Bar-Am, O., Epsztejn, S., Cabantchik, Z. I., Warshawsky, A., Youdim, M. B. H. & Fridkin, M. (2005). *Bioorg. Med. Chem.* **13**, 773–783.