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N-Benzylquinoline-8-sulfonamide

Carla Regina Andrighetti-Fröhner,[a,b] Luiz Everson da Silva,[a] Ricardo José Nunes,[a,b] Cláudia Maria Oliveira Simões[c] and Sabine Foro[b]*

[a]Departamento de Química–UFSC, 88040-900 Florianópolis, SC, Brazil, [b]Clemens Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany, and [c]Departamento de Ciências Farmacêuticas–UFSC, 88040-900 Florianópolis, SC, Brazil

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 = 0.078
wR factor = 0.236
Data-to-parameter ratio = 13.2

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

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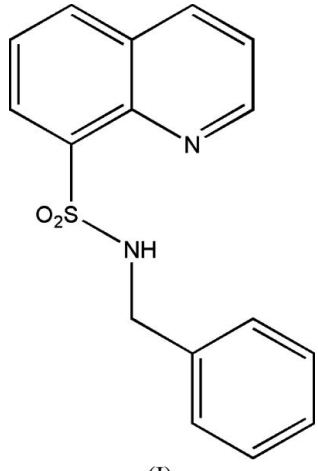
In the title compound, $C_{16}H_{14}N_2O_2S$, the C—N—S—C torsion angle is −63.1 (4)°. One intramolecular N—H···N hydrogen bond is observed in the structure.

Comment

Quinoline and its derivatives comprise an important class of heterocyclic compounds present in many biologically active molecules such as multi-drug-resistant cancer cells (Gao *et al.*, 1999) and have demonstrated antibacterial activity (Patel & Patel, 1999). In addition, quinoline derivatives have been reported to show broad-spectrum efficacy against multiple herpes viruses and they may have a potential role in 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 a project to investigate the structure–function relationships and develop more effective antiviral drugs (Andrigetti-Fröhner *et al.*, 2003), we report here the crystal structure of the title compound, (I).



(I)

The key feature of the molecular structure of (I) (Fig. 1) is the C10—N1—S1—C1 torsion angle of −63.1 (4)°, which illustrates the non-planarity of the molecule. The H atom of the NH group has an intramolecular contact with the N atom of the quinoline ring system (Table 1).

Experimental

The title compound was prepared by the reaction of 1 equivalent of 8-quinolinesulfonyl chloride (1 mmol) and benzylamine (2 mmol) in the presence of methanol (5 ml) for 2 h, at room temperature,

according to the literature procedure of Buchmann & Schalinatus (1962). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from a methanol/dichloromethane solution (1:1).

Crystal data

$C_{16}H_{14}N_2O_2S$
M_r = 298.35
Monoclinic, $P2_1/n$
a = 10.142 (2) Å
b = 9.980 (2) Å
c = 14.428 (2) Å
β = 100.25 (2)°
V = 1437.1 (5) Å^3
Z = 4
D_x = 1.379 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.05 mm^{-1}
T = 299 (2) K
Block, yellow
0.55 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.532, T_{max} = 0.611
(expected range = 0.470–0.540)
2649 measured reflections
2546 independent reflections
2203 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 66.8°
3 standard reflections
frequency: 120 min
intensity decay: 1.3%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.078
$wR(F^2)$ = 0.236
S = 1.10
2546 reflections
193 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1508P)^2 + 0.7674P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.80 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*N*···N2	0.84 (5)	2.32 (5)	2.929 (5)	130 (4)

The H atom of the NH group was located in a difference map and its position refined. The carbon-bound H atoms were positioned with idealized geometry, with C—H distances in the range 0.93–0.97 Å and refined using a riding model. Isotropic displacement parameters for all H atoms were set equal to $1.2U_{eq}$(parent atom).

Data collection: *CAD-4-PC* (Enraf–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: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

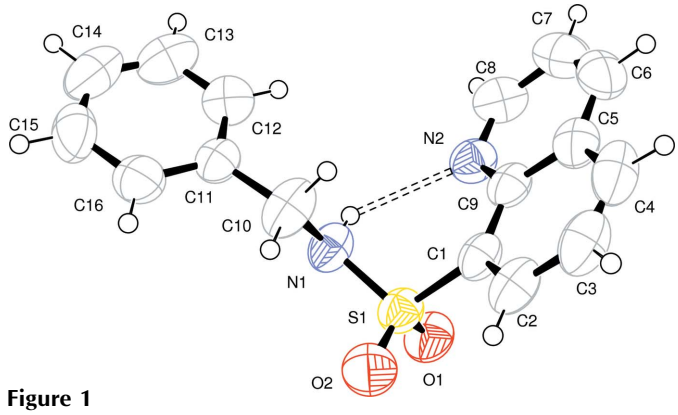


Figure 1
The molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level. The intramolecular hydrogen bond is shown dashed.

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