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Key indicators

Single-crystal X-ray study
T = 299 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
Disorder in main residue
R factor = 0.044
wR factor = 0.132
Data-to-parameter ratio = 12.8

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

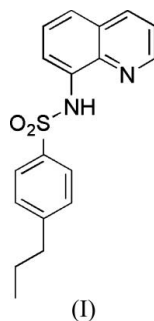
4-*n*-Propyl-*N*-(8-quinoly)benzenesulfonamide

In the title compound, $\text{C}_{18}\text{H}_{18}\text{N}_2\text{O}_2\text{S}$, the torsion angle about the N–S bond between the quinoline ring system and the benzene ring is $-60.9(2)^\circ$. The NH group forms an intramolecular hydrogen bond to the quinoline N atom.

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Comment

Zinc(II)-specific fluorophores are of substantial importance in the study of intracellular Zn^{2+} . Various fluorescence-based quinoline cores are currently the most widely used zinc-activated fluorophores (Frederickson *et al.*, 1987; Savage *et al.*, 1989; Kimber *et al.*, 2000). We report here the structure of the title compound, (I), determined as part of our studies to investigate potential new fluorophores to be used as ligands for coordination to Zn^{II} and Cu^{II} ions (da Silva *et al.*, 2005*a,b,c,d,e*, 2006).



The quinoline ring system forms a C1–N1–S1–C10 torsion angle with the benzene ring of $-60.9(2)^\circ$, indicating non-planarity in the molecule. The NH group forms an intramolecular hydrogen bond to the quinoline N atom (Table 1).

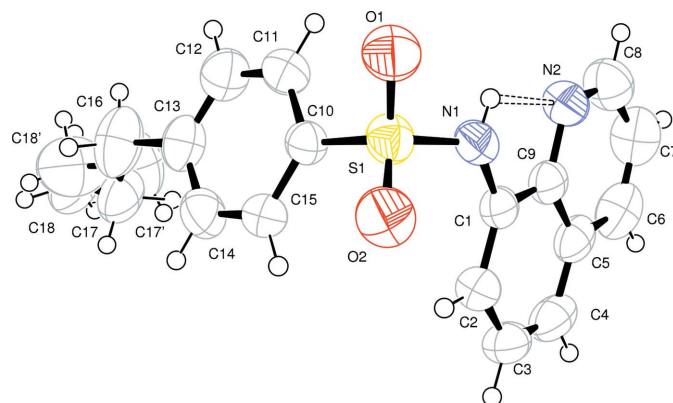


Figure 1

The molecular structure of (I), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level. Both disorder components are shown. The hydrogen bonding is shown as dashed lines.

Experimental

Compound (I) was prepared by according to the literature procedure of Xue *et al.* (2000). Suitable crystals were obtained by recrystallization from methanol–dichloromethane (1:1) (m.p. 378 K).

Crystal data

$C_{18}H_{18}N_2O_2S$	$Z = 4$
$M_r = 326.40$	$D_x = 1.312 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation
$a = 6.7242 (8) \text{ \AA}$	$\mu = 1.83 \text{ mm}^{-1}$
$b = 14.031 (1) \text{ \AA}$	$T = 299 (2) \text{ K}$
$c = 17.513 (1) \text{ \AA}$	Block, colourless
$\beta = 90.891 (9)^\circ$	$0.50 \times 0.30 \times 0.17 \text{ mm}$
$V = 1652.1 (2) \text{ \AA}^3$	

Data collection

Nonius CAD-4 diffractometer	2431 reflections with $I > 2\sigma(I)$
$\omega/2\theta$ scans	$R_{\text{int}} = 0.051$
Absorption correction: ψ scan	$\theta_{\text{max}} = 66.9^\circ$
(North <i>et al.</i> , 1968)	3 standard reflections
$T_{\text{min}} = 0.546$, $T_{\text{max}} = 0.723$	frequency: 120 min
6255 measured reflections	intensity decay: 1.5%
2933 independent reflections	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0681P)^2 + 0.3991P]$
$R[F^2 > 2\sigma(F^2)] = 0.044$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.133$	$(\Delta/\sigma)_{\text{max}} = 0.002$
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.34 \text{ e \AA}^{-3}$
2933 reflections	$\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$
230 parameters	Extinction correction: <i>SHELXL97</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0079 (7)

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1N\cdots N2$	0.80 (3)	2.19 (3)	2.651 (3)	117 (2)

The H atom of the NH group was located in a difference map and its position refined [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$]. The carbon-bound H atoms

were positioned with idealized geometry and refined using a riding model, with C–H distances in the range 0.93–0.97 \AA and isotropic displacement parameters set at 1.2 times U_{eq} value of the parent atom. Atoms C17 and C18 of the propyl group are disordered and were refined with a split model. The corresponding site-occupation factors were refined but later fixed at 0.5:0.5.

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: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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