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2-(1,3-Benzothiazol-2-yl)quinolin-8-ol

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.093
Data-to-parameter ratio = 10.8

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

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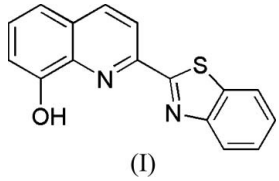
The molecules of the title compound, $C_{16}H_{10}N_2OS$, are nearly planar. An intramolecular O—H···N and an intermolecular C—H···O hydrogen bond are obseved in the crystal structure.

Comment

8-Hydroxyquinoline derivatives show a wide spectrum of properties as analytical reagents, due to their ability to form stable complexes with many metallic ions (Bratzel *et al.*, 1972). On the other hand, organic fluorophores have received much attention in recent years because of their applications in the optoelectronics industry as well as in the treatment of Alzheimer's disease (Ooyama *et al.*, 2005; Raman *et al.*, 2005).



(I)

As part of our ongoing search for fluorophores based on a clioquinol system as a potential fluorophore for neurodegenerative diseases (Padmanabhan *et al.*, 1989), we report here the structure of the title compound, (I). The molecules are nearly planar (r.m.s. deviation for all atoms = 0.025 Å). The OH group forms an intramolecular hydrogen bond to the quinoline N atom. In addition, an intermolecular C—H···O hydrogen bond connects the molecules into a three-dimensional network, as shown in the packing diagram (Fig. 2). Details of these hydrogen bonds are given in Table 1.

Experimental

The title compound was prepared according to the procedure described by Chen (2005). Single crystals suitable for X-ray data

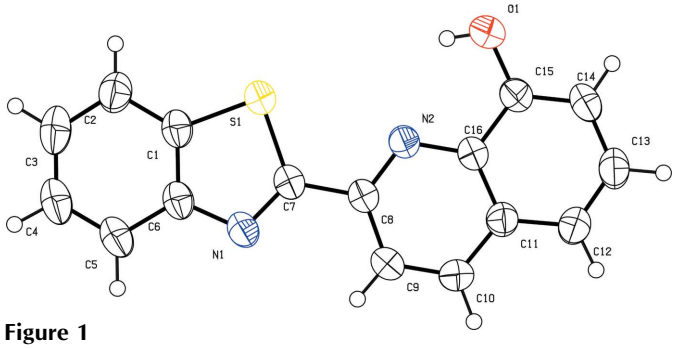


Figure 1
The molecular structure of (I), showing the atom labeling; displacement ellipsoids are drawn at the 50% probability level.

collection were obtained by recrystallization from dichloromethane–hexane (1:1 *v*/*v*).

Crystal data

$C_{16}H_{10}N_2OS$
M_r = 278.32
Monoclinic, $C2/c$
a = 12.182 (2) Å
b = 8.0602 (8) Å
c = 26.061 (3) Å
β = 91.53 (1)°
V = 2558.0 (6) Å^3
Z = 8
D_x = 1.445 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 6.5–21.1°
μ = 2.21 mm^{-1}
T = 299 (2) K
Prism, light brown
0.35 × 0.20 × 0.13 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.626, T_{max} = 0.760
3228 measured reflections
2282 independent reflections
1918 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 66.9°
$h = 0 \rightarrow 14$
$k = -9 \rightarrow 3$
$l = -31 \rightarrow 31$
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.093
S = 1.05
2282 reflections
211 parameters
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0497P)^2 + 1.0455P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.011
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*O*···N2	0.81 (3)	2.18 (3)	2.6859 (19)	121 (2)
C12—H12···O1^{i}	0.96 (2)	2.51 (2)	3.348 (3)	145.6 (18)

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

All H atoms were located in a difference map and their coordinates were refined with isotropic displacement parameters set to 1.2U_{eq}(parent atom).

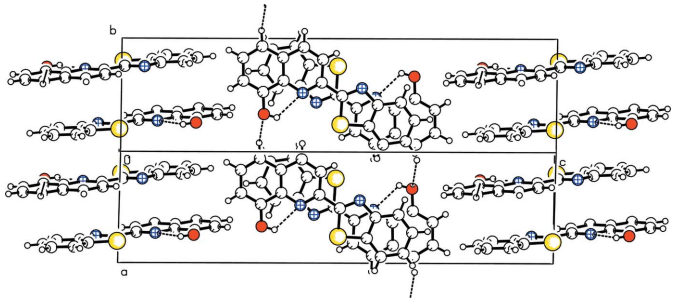


Figure 2
Packing diagram of (I), with hydrogen bonds shown as dashed lines.

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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