

## 5-(4-Ethoxyphenyldiazenyl)-8-hydroxyquinoline

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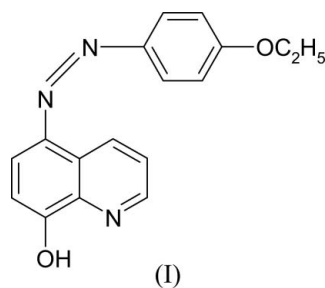
## Key indicators

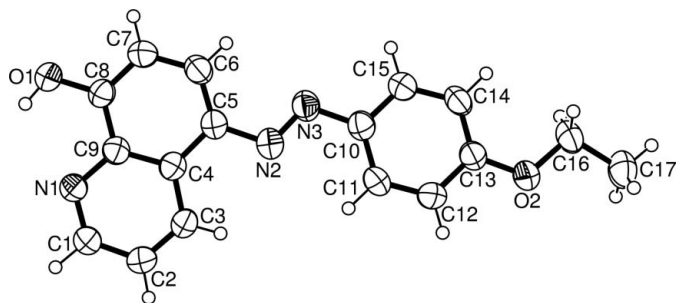
Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(C-C) = 0.004$  Å  
 $R$  factor = 0.113  
 $wR$  factor = 0.205  
Data-to-parameter ratio = 17.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

In the molecules of the title compound,  $C_{17}H_{15}N_3O_2$ , the ethoxyphenyl ring forms a dihedral angle of  $7.37$  ( $11^\circ$ ) with the quinoline ring system. In the crystal structure, intermolecular  $O-H \cdots N$  hydrogen bonds link the molecules into centrosymmetric  $R_2^2(10)$  dimers; these dimers are arranged in sheets parallel to the  $ab$  plane.

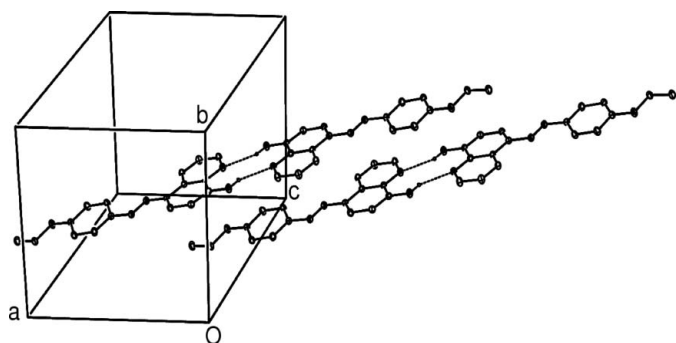
## Comment

The chemical properties of quinoline and its derivatives have been widely discussed because of their biological relevance, coordination capacity and their use as metal-extracting agents (Shoair *et al.*, 2001). They have attracted special interest due to their therapeutic properties. Quinoline sulfonamides have been used in the treatment of cancer, tuberculosis and malaria (El-Sonbati *et al.*, 2001). Several quinoline derivatives possess chemotherapeutic activity and act as antimalaria and anti-allergic agents (Mekheimer *et al.*, 1998). They show broad-spectrum efficiency against multiple herpes viruses and have a potential role in the treatment of a variety of infections (Hartline *et al.*, 2005). 8-Hydroxyquinoline and its derivatives have high antibacterial activities (Deb & Ghosh, 1987). Some of its derivatives and their complexes with transition metals have been reported to be active against some bacteria (Zidan, 2002). In addition, azo compounds based on 8-hydroxyquinoline derivatives play a central role as chelating agents for a large number of metal ions (La Deda *et al.*, 2004). In recent years, a number of novel merocyanine dyes have been synthesized which contain the 8-hydroxyquinoline nucleus and these dyes exhibit strong metallochromic behavior against some heavy and transition metal ions (Kovtun *et al.*, 2004). Some 8-hydroxyquinoline and azo derivatives have found numerous applications in analytical chemistry as chromophoric and metallochromic indicators (Hadi, 1994). This study was undertaken in order to ascertain the crystal structure of the title phenyldiazenylquinoline dye, (I).

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



**Figure 2**  
Partial packing diagram of (I), showing hydrogen-bonded (dashed lines) dimers. H atoms not involved in hydrogen bonds have been omitted.

quinoline units. The bond lengths and angles (Table 1) are in normal ranges (Allen *et al.*, 1987).

The quinoline ring system is planar, the dihedral angle between the N1/C1–C4/C9 and C4–C9 rings being 1.60 (14)°. The C10–C15 benzene ring is oriented at a dihedral angle of 7.37 (11)° with respect to the quinoline ring system. The phenyldiazenyl unit is nearly planar.

As can be seen from the packing diagram (Fig. 2), intermolecular O–H...N [H1...N1<sup>i</sup> 2.16 (5), O1...N1<sup>i</sup> 2.879 (3) Å and O1–H1...N1<sup>i</sup> 141 (4)°; symmetry code: (i) 2 – x, 2 – y, –z] hydrogen bonds link the molecules into dimers, which are stacked along the *b* axis, forming a layer parallel to the *ab* plane. Dipole–dipole and van der Waals interactions are effective in the molecular packing.

## Experimental

4-Ethoxyaniline (0.27 g, 2 mmol) was dissolved in HCl (1.5 ml) and water (4.0 ml). The solution was cooled in an ice–salt bath and a cold solution of NaNO<sub>2</sub> (0.15 g, 2 mmol) in water (3.0 ml) was added dropwise with stirring. The resulting diazonium salt was also cooled in an ice–salt bath and then added dropwise with stirring to 8-hydroxyquinoline (0.29 g, 2 mmol) in an aqueous solution of KOH (2 mmol, 15 ml). The resulting solution was stirred at 273–278 K for 1 h and the pH of the reaction mixture was maintained at 4–6 by the simultaneous addition of a saturated sodium acetate solution (15–20 ml). The mixture was stirred for a further 1 h. The resulting solid

was filtered off, washed with cold water and recrystallized from toluene (yield 0.45 g, 85%; m.p. 455–456 K).

## Crystal data

C<sub>17</sub>H<sub>15</sub>N<sub>3</sub>O<sub>2</sub>  
M<sub>r</sub> = 293.32  
Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 10.5985 (3) Å  
*b* = 11.2970 (2) Å  
*c* = 12.7652 (3) Å  
 $\beta$  = 107.697 (1)°  
*V* = 1456.07 (6) Å<sup>3</sup>

*Z* = 4  
*D<sub>x</sub>* = 1.338 Mg m<sup>−3</sup>  
Mo K $\alpha$  radiation  
 $\mu$  = 0.09 mm<sup>−1</sup>  
*T* = 296 (2) K  
Block, orange  
0.35 × 0.25 × 0.15 mm

## Data collection

Rigaku R-AXIS RAPID-S  
diffractometer  
 $\omega$  scans  
Absorption correction: none  
42707 measured reflections

4447 independent reflections  
2715 reflections with *I* > 2 $\sigma$ (*I*)  
*R*<sub>int</sub> = 0.097  
 $\theta$ <sub>max</sub> = 30.6°

## Refinement

Refinement on *F*<sup>2</sup>  
*R* [*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.114  
*wR* (*F*<sup>2</sup>) = 0.205  
*S* = 1.24  
4447 reflections  
248 parameters  
H atoms treated by a mixture of  
independent and constrained  
refinement

$w = 1/[\sigma^2(F_o^2) + (0.0448P)^2 + 0.5792P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
( $\Delta/\sigma$ )<sub>max</sub> = 0.001  
 $\Delta\rho$ <sub>max</sub> = 0.16 e Å<sup>−3</sup>  
 $\Delta\rho$ <sub>min</sub> = −0.28 e Å<sup>−3</sup>

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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