

9-[Ethoxy(8-quinolylamino)methyl]anthracene

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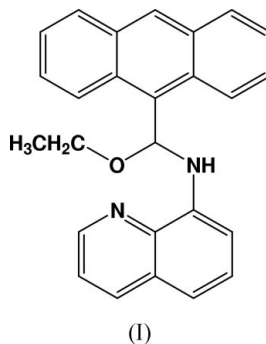
Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(C-C) = 0.003$ Å
 R factor = 0.050
 wR factor = 0.152
Data-to-parameter ratio = 14.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $C_{26}H_{22}N_2O$, was readily synthesized from the reaction between 8-aminoquinoline and 9-anthraldehyde in EtOH solution. There is an intramolecular N—H···N hydrogen bond and weak C—H···N/O interactions. The molecule self-assembles into a zigzag chain along the c axis through π – π interactions.

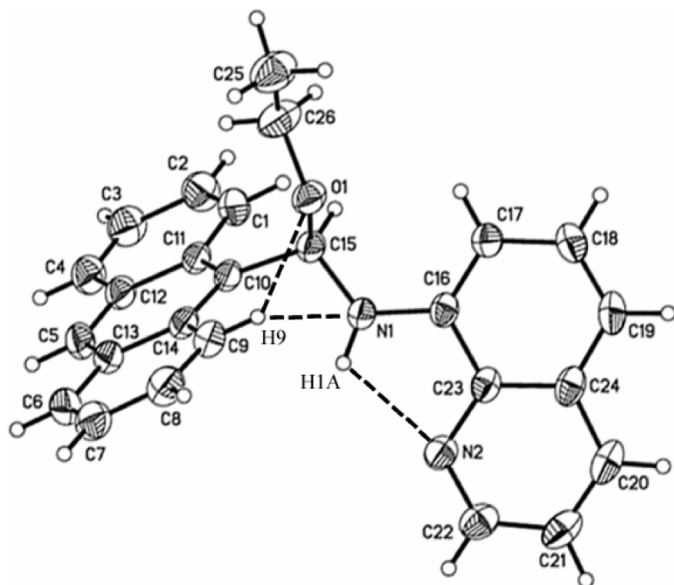
Comment

In the pharmaceutical industry, much research has been conducted in recent years on enantiomerically pure compounds, in order to discover and develop safer and more efficacious drugs (Liu *et al.*, 1997; Bolender & Richardson, 2003). Moreover, most of today's top-selling drugs are optically pure enantiomers (Maier *et al.*, 2001). Many racemic compounds which belong to the 8-aminoquinoline class of agents are used as effective antimalarial drugs (Vangapandu *et al.*, 2004; Jain *et al.*, 2004), and continuous research efforts have been devoted to reducing the drawbacks of these drugs while improving their activities (Vangapandu *et al.*, 2004). It is very important to study the crystal structures of 8-aminoquinoline derivatives as well, to check the activity of these medicines in order to understand the structure–function relationships and develop more effective antimalarial drugs. We report here the crystal structure of the title compound, (I), which is a new 8-aminoquinoline derivative.



The molecular structure of (I) is illustrated in Fig. 1. It has a chiral carbon center, C15, but the compound is racemic. There is an intramolecular N—H···N hydrogen bond and C—H···N/O weak interactions (Table 2). The dihedral angle between the anthracene and quinoline ring systems is $70.61(3)^\circ$. The molecular packing of (I) is shown in Fig. 2. Zigzag chains of molecules are formed along the c axis through the π – π interactions of the two ring systems of neighboring anthracene [$Cg1 \cdots Cg1^i = 3.81(3)$ Å] and adjacent aminoquinoline [$Cg2 \cdots Cg2^{ii} = 3.80(3)$ Å], $Cg1$ and $Cg2$ being the centers of the C11–C12 and C23–C24 bonds,

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Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids with the atom-numbering scheme. Dashed lines indicate hydrogen bonds and weak C—H...X interactions.

respectively [symmetry codes: (i) $2 - x, 1 - y, 2 - z$; (ii) $2 - x, 1 - y, 1 - z$].

Experimental

To an ethanol solution (8 ml) of 8-aminoquinoline (0.577 g, 4 mmol) was added 9-anthraldehyde (0.833 g, 4 mmol) with stirring. The resulting solution was heated under reflux for 1 h and then filtered. The resulting yellow precipitate was dissolved in EtOH (15 ml) with heating and then filtered off. The filtrate was left at room temperature and yellow crystals of (I) were deposited after 24 h (yield 76%). Analysis calculated: C 82.51, H 5.86, N 7.40%; found: C 82.75, H 5.76, N 7.51%. IR (KBr, cm^{-1}): 3340.1 [$m, \nu(\text{N—H})$], 3046.7 [$w, \nu(\text{C—H})$], 2973.5 [$w, \nu(\text{—CH}_2\text{—})$], 2883.6 [$w, \nu(\text{—CH}_2\text{—})$], 1622.8 [$w, \nu(\text{C=C})$], 1574.5 [$m, \nu(\text{C—H})$], 1515.8 [$s, \nu(\text{=C—H})$], 1475.6 [$m, \nu(\text{—CH}_2\text{—})$], 1444.5 [$w, \nu(\text{=C—H})$], 1380.2 [$m, \delta(\text{—C—H})$], 1331.2 [$m, \nu(\text{C—N})$], 1153.8 [$w, \delta(\text{=C—H})$], 1065.9 [$m, \nu(\text{C—O—C})$], 986.7 [$m, \gamma(\text{=C—H})$], 884.2 [$w, \gamma(\text{=C—H})$], 816.7 [$w, \gamma(\text{=C—H})$], 788.3 [$m, \gamma(\text{=C—H})$], 742.6 [$w, \gamma(\text{=C—H})$], 731.1 [$m, \gamma(\text{=C—H})$].

Crystal data

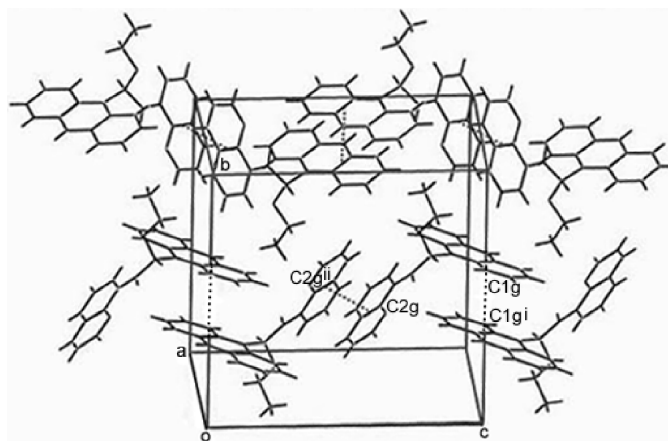
$\text{C}_{26}\text{H}_{22}\text{N}_2\text{O}$
 $M_r = 378.46$
 Monoclinic, $P2_1/n$
 $a = 9.268$ (2) Å
 $b = 14.595$ (2) Å
 $c = 14.466$ (2) Å
 $\beta = 90.09$ (1)°
 $V = 1956.8$ (6) Å³
 $Z = 4$

$D_x = 1.285$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 3698 reflections
 $\theta = 2.6\text{--}26.1^\circ$
 $\mu = 0.08$ mm⁻¹
 $T = 293$ (2) K
 Hexagonal prism, yellow
 $0.3 \times 0.2 \times 0.2$ mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan [SADABS (Sheldrick, 1996) in SAINT (Bruker, 2000)]
 $T_{\min} = 0.979, T_{\max} = 0.982$
 10 778 measured reflections

3873 independent reflections
 2684 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 26.1^\circ$
 $h = -10 \rightarrow 11$
 $k = -18 \rightarrow 18$
 $l = -17 \rightarrow 12$


Figure 2

The crystal structure of (I). Broken lines indicate π – π interactions. [Symmetry codes: (i) $2 - x, 1 - y, 2 - z$; (ii) $2 - x, 1 - y, 1 - z$.]

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.050$
 $wR(F^2) = 0.152$
 $S = 1.07$
 3873 reflections
 275 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0885P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.19 \text{ e \AA}^{-3}$

Table 1

Selected torsion angles (°).

C14—C10—C15—N1	61.75 (18)	C17—C16—N1—C15	15.5 (3)
N1—C16—C23—N2	1.4 (2)	C10—C15—N1—C16	162.47 (15)

Table 2

Hydrogen-bonding geometry (Å, °).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
N1—H1A...N2	0.892 (17)	2.203 (17)	2.663 (2)	112 (1)
C9—H9...O1	0.93	2.375	2.956 (2)	120
C9—H9...N1	0.93	2.587	3.030 (2)	110

Atoms H1A and H15 were located in difference Fourier maps, and refined isotropically, the N1—H1A and C15—H15 distances being 0.892 (17) Å and 0.955 (17) Å, respectively. The remaining H atoms were positioned geometrically and refined as riding, with C—H distances of 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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