Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4,6-Dimethyl-2-(*o*-tolyliminomethyl)quinoline

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.073
wR factor = 0.187
Data-to-parameter ratio = 17.6

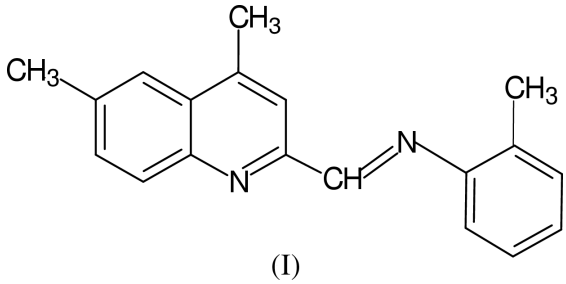
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 18 April 2001
Accepted 20 April 2001
Online 30 April 2001

The molecule of the title compound, $C_{19}H_{18}N_2$, is not planar. The dihedral angle between the quinoline and phenyl rings is 118.5 (1)°.

Comment

Interest in quinoxaline derivatives has increased greatly during recent years due to their different applications in various areas. Some derivatives are used as colorimetric agents (Campaigne & McLaughlin, 1983), antibacterial agents (Boutti & Lecolier, 1976) and colouring matter. Other derivatives possess various biological activities (De Clercq, 1998; Li *et al.*, 1997). Much attention has recently been concentrated on compounds obtained from heterocyclic carbaldehydes for the treatment of cancer (Kouznetsov *et al.*, 1998; Öcal & Kaban, 1998). The structure of 4,6-dimethyl-2-(*o*-tolyliminomethyl)quinoline, (I), has been determined and is presented here.



(I)

The quinoline and phenyl rings are planar. In the quinoline ring, the angle C3—C4—C5 is greater than 120° [123.4 (2)°] and the angle C8—C9—N1 is smaller than 120° [118.2 (2)°] (Öztürk *et al.*, 2000). The dihedral angle between the least-squares planes of the quinoline and phenyl rings is 118.5 (1)°.

Experimental

The title compound was synthesized by the condensation of 4,6-dimethylquinoline-2-carbaldehyde with *o*-toluidine in dry ethanol for 6.5 h. Light-yellow crystals were obtained after crystallization from ethanol. Yield: 54%; m.p.: 392 K; IR (KBr): γ 3040, 2890, 1585 cm^{-1}; ^{1}H NMR ($CDCl_3$, δ, 200 MHz): 2.46 (3H, *s*, *o*-CH_3), 2.59 (3H, *s*, 6-CH_3), 2.76 (3H, *s*, 4-CH_3), 7.05–8.64 (9H, *m*, ArH and CH) p.p.m.; UV ($CHCl_3$): λ_{max} 260.8, 312.5 nm. Elemental analysis, $C_{19}H_{18}N_2$ requires: C 83.18, H 6.61, N 10.21%; found: C 83.14, H 6.58, N 10.11% (Aydoğan, 1993).

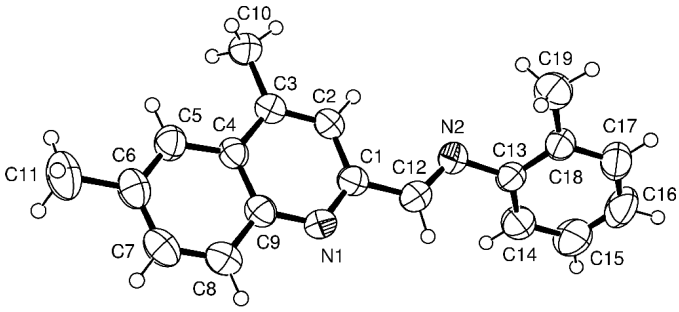


Figure 1
An *ORTEP*II drawing of the molecular structure of (I) showing the labelling of the non-H atoms. Anisotropic displacement ellipsoids are shown at the 50% probability level.

Crystal data

$C_{19}H_{18}N_2$
$M_r = 274.37$
Triclinic, $P\overline{1}$
$a = 7.5693$ (7) Å
$b = 9.5620$ (9) Å
$c = 11.3908$ (11) Å
$\alpha = 79.203$ (2)°
$\beta = 76.735$ (2)°
$\gamma = 77.514$ (2)°
$V = 775.19$ (13) Å^3
$Z = 2$
$D_x = 1.180$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1739 reflections
$\theta = 3.1$–27.5°
$\mu = 0.07$ mm^{-1}
$T = 293$ (2) K
Needle, colourless
0.44 × 0.26 × 0.06 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
5000 measured reflections
3414 independent reflections
1697 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 27.5°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.073$
$wR(F^2) = 0.236$
$S = 1.02$
3414 reflections
194 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1124P)^2 + 0.0410P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.24$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: *SHELXL*93
Extinction coefficient: 0.023 (9)

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.316 (3)	C3—C10	1.496 (4)
N1—C9	1.364 (3)	C6—C11	1.515 (4)
N2—C12	1.267 (3)	C18—C19	1.501 (4)
N2—C13	1.420 (3)		
C1—N1—C9	118.0 (2)	C5—C6—C11	120.2 (3)
C12—N2—C13	119.0 (2)	C7—C6—C11	120.9 (3)
C2—C3—C10	121.2 (2)	N1—C9—C8	118.2 (2)
C4—C3—C10	121.8 (2)	C17—C18—C19	121.3 (3)
C5—C4—C3	123.4 (2)	C13—C18—C19	120.7 (3)
C13—N2—C12—C1	−178.6 (2)		

The methyl groups were allowed to rotate about their local threefold axes.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *ORTEP*II (Johnson, 1976).

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