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6-Methyl-3-*p*-tolyl-3,4-dihydroquinazoline

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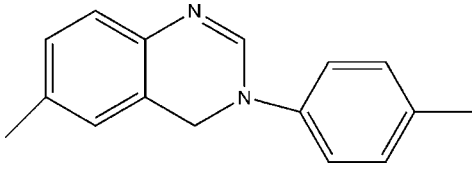
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.076; wR factor = 0.200; data-to-parameter ratio = 15.8.

In the molecule of the title compound, $C_{16}H_{16}N_2$, the dihedral angles between the the two benzene rings is 14.7 (1)°; the heterocyclic ring is slightly puckered, the maximum deviation from the plane of the fused benzene ring being 0.262 (4) Å for the N atom attached to the tolyl ring. In the crystal structure, van der Waals forces link the molecules into layers which are stacked along the *a* and *b* axes.

Related literature

For related literature, see: Allen *et al.* (1987); Connolly *et al.* (2005).



Experimental

Crystal data

$C_{16}H_{16}N_2$
M_r = 236.31
Monoclinic, $P2_1/a$
a = 6.2745 (7) Å
b = 14.6008 (15) Å
c = 14.0154 (11) Å
β = 94.39 (3)°
V = 1280.2 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.50 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.965, T_{max} = 0.993
2739 measured reflections
2500 independent reflections
1294 reflections with $I > 2\sigma(I)$
R_{int} = 0.082
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.076
$wR(F^2)$ = 0.200
S = 1.07
2500 reflections
158 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RT2006).

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supplementary materials

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6-Methyl-3-*p*-tolyl-3,4-dihydroquinazoline

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Comment

Quinazolines is a class of fused heterocycles that are of considerate interest because of the diverse range of their biological properties, for example, anticancer, diuretic, anti-inflammatory, anticonvulsant and antihypertensive activities (Connolly *et al.*, 2005).

In the molecule of (I), (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angles between the planar rings A (C2–C7), B (C4/C5/C8/C9/N1/N2) and C (C10–C15) are A/B = 4.8 (1)°, B/C = 11.9 (1)° and A/C = 14.7 (1)°.

As can be seen from the packing diagram (Fig. 2), the molecules of (I) are formed into layers which are stacked along the *a* axis and *b* axis.

Experimental

p-toluidine (AR) (10.7 g,0.1 mol) and distilled water (300 ml) were added into the four-neck round-bottom flask fitted with a mechanical stirrer, dropping funnel, thermometer, and reflux condenser. The mixture was kept at 298 K under nitrogen. Then chlorhydric acid (AR) (37%, 12.6 ml) was added dropwise maintaining carefully the temperature and stirring. 30 min later, the reaction mixture was warmed up to 313 K and formaldehyde solution (37%, 3.8 ml) was added dropwise. The following 2 h the mixture was stirred at 323 K then 2 h at 373 K. On cooling, the mixture was neutralized with sodium hydroxide solution (1%, 50 ml) to pH 6 and filated. The filate was slowly neutralized to pH 7 with sodium hydroxide solution. Solvent and *p*-toluidine were distilled under reduced pressure. The product was purified by repeated crystallization. Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of ethyl ether. (yield; 8.5 g, 36%, m.p. 435 K)

Refinement

H atoms were positioned geometrically, with C—H = 0.93, 0.93, 0.96 and 0.97 Å for aromatic, methenyl, methyl, methylene respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

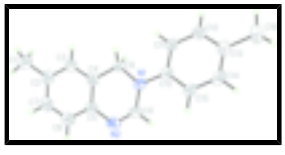

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Fig. 2. A packing diagram for (I).

6-Methyl-3-*p*-tolyl-3,4-dihydroquinazoline

Crystal data

$C_{16}H_{16}N_2$	F_{000} = 504
M_r = 236.31	D_x = 1.226 Mg m^{-3}
Monoclinic, $P2_1/a$	Melting point: 435 K
Hall symbol: -P 2yab	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.2745 (7) Å	Cell parameters from 25 reflections
b = 14.6008 (15) Å	θ = 10–13º
c = 14.0154 (11) Å	μ = 0.07 mm^{-1}
β = 94.39 (3)º	T = 298 (2) K
V = 1280.2 (2) Å^3	Plate, yellow
Z = 4	0.50 × 0.30 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.082
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 2.0º
T = 298(2) K	h = −7→7
ω/2θ scans	k = 0→17
Absorption correction: ψ scan (North *et al.*, 1968)	l = 0→17
T_{min} = 0.965, T_{max} = 0.993	3 standard reflections
2739 measured reflections	every 200 reflections
2500 independent reflections	intensity decay: none
1294 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.076	H-atom parameters constrained
$wR(F^2)$ = 0.200	$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + 0.7P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.07	$(\Delta/\sigma)_{max} < 0.001$
2500 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
158 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Primary atom site location: structure-invariant direct methods

Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.6678 (4)	0.38190 (17)	0.57235 (17)	0.0510 (7)
N2	1.0036 (4)	0.4135 (2)	0.6578 (2)	0.0704 (8)
C1	0.6452 (7)	0.3515 (3)	1.0142 (3)	0.098
H1A	0.7489	0.3663	1.0658	0.147*
H1B	0.6026	0.2887	1.0194	0.147*
H1C	0.5225	0.3904	1.0172	0.147*
C2	0.7421 (7)	0.3660 (3)	0.9198 (2)	0.0775 (11)
C3	0.6227 (6)	0.3486 (2)	0.8341 (2)	0.0661 (9)
H3A	0.4846	0.3258	0.8355	0.079*
C4	0.7041 (5)	0.3645 (2)	0.7467 (2)	0.0556 (8)
C5	0.9117 (5)	0.3963 (2)	0.7451 (2)	0.0593 (9)
C6	1.0329 (6)	0.4132 (3)	0.8300 (3)	0.0759 (11)
H6A	1.1719	0.4349	0.8287	0.091*
C7	0.9484 (7)	0.3978 (3)	0.9161 (3)	0.0805 (12)
H7A	1.0314	0.4091	0.9727	0.097*
C8	0.5695 (5)	0.3451 (2)	0.6562 (2)	0.0570 (8)
H8A	0.5510	0.2794	0.6490	0.068*
H8B	0.4294	0.3723	0.6600	0.068*
C9	0.8787 (5)	0.4058 (2)	0.5816 (3)	0.0649 (9)
H9A	0.9401	0.4183	0.5247	0.078*
C10	0.5485 (5)	0.3786 (2)	0.4822 (2)	0.0512 (8)
C11	0.3519 (5)	0.3348 (2)	0.4725 (2)	0.0561 (8)
H11A	0.2965	0.3090	0.5260	0.067*
C12	0.2370 (5)	0.3290 (2)	0.3845 (2)	0.0607 (9)
H12A	0.1062	0.2987	0.3799	0.073*
C13	0.3117 (6)	0.3670 (2)	0.3029 (2)	0.0625 (9)
C14	0.5045 (6)	0.4121 (2)	0.3141 (2)	0.0699 (10)
H14A	0.5584	0.4385	0.2606	0.084*
C15	0.6217 (6)	0.4200 (2)	0.4012 (2)	0.0651 (9)
H15A	0.7491	0.4528	0.4058	0.078*
C16	0.1841 (7)	0.3585 (3)	0.2075 (2)	0.0905 (13)

H16A	0.2119	0.4105	0.1683	0.136*
H16B	0.0345	0.3561	0.2173	0.136*
H16C	0.2249	0.3035	0.1761	0.136*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0463 (14)	0.0517 (15)	0.0562 (16)	−0.0031 (12)	0.0128 (12)	0.0006 (12)
N2	0.0509 (16)	0.083 (2)	0.077 (2)	−0.0094 (15)	0.0073 (15)	−0.0031 (17)
C1	0.098	0.098	0.098	0.000	0.007	0.000
C2	0.086 (3)	0.090 (3)	0.056 (2)	0.008 (2)	0.003 (2)	0.005 (2)
C3	0.062 (2)	0.078 (2)	0.059 (2)	−0.0011 (19)	0.0030 (17)	0.0060 (18)
C4	0.0507 (18)	0.057 (2)	0.0590 (19)	0.0032 (16)	0.0029 (15)	−0.0011 (16)
C5	0.0493 (18)	0.057 (2)	0.071 (2)	0.0006 (16)	0.0029 (17)	−0.0057 (17)
C6	0.061 (2)	0.076 (3)	0.089 (3)	−0.001 (2)	−0.006 (2)	−0.007 (2)
C7	0.079 (3)	0.087 (3)	0.073 (3)	0.006 (2)	−0.013 (2)	−0.005 (2)
C8	0.0528 (19)	0.062 (2)	0.0576 (19)	−0.0080 (16)	0.0136 (16)	0.0025 (16)
C9	0.054 (2)	0.071 (2)	0.073 (2)	−0.0104 (18)	0.0173 (18)	−0.0031 (19)
C10	0.0555 (19)	0.0459 (17)	0.0530 (18)	0.0000 (15)	0.0096 (15)	−0.0011 (14)
C11	0.060 (2)	0.061 (2)	0.0476 (18)	−0.0044 (17)	0.0119 (15)	0.0051 (15)
C12	0.060 (2)	0.059 (2)	0.062 (2)	−0.0036 (17)	0.0060 (17)	−0.0002 (17)
C13	0.081 (2)	0.0503 (19)	0.056 (2)	0.0079 (18)	0.0074 (18)	0.0021 (16)
C14	0.092 (3)	0.063 (2)	0.058 (2)	−0.007 (2)	0.021 (2)	0.0101 (17)
C15	0.068 (2)	0.061 (2)	0.068 (2)	−0.0119 (18)	0.0167 (18)	0.0080 (17)
C16	0.117 (3)	0.093 (3)	0.059 (2)	0.006 (3)	−0.003 (2)	−0.002 (2)

Geometric parameters (Å, °)

N1—C9	1.365 (4)	C7—H7A	0.9300
N1—C10	1.419 (4)	C8—H8A	0.9700
N1—C8	1.471 (4)	C8—H8B	0.9700
N2—C9	1.280 (4)	C9—H9A	0.9300
N2—C5	1.414 (4)	C10—C11	1.387 (4)
C1—C2	1.512 (5)	C10—C15	1.395 (4)
C1—H1A	0.9600	C11—C12	1.384 (4)
C1—H1B	0.9600	C11—H11A	0.9300
C1—H1C	0.9600	C12—C13	1.384 (4)
C2—C7	1.380 (5)	C12—H12A	0.9300
C2—C3	1.390 (5)	C13—C14	1.376 (5)
C3—C4	1.381 (4)	C13—C16	1.510 (5)
C3—H3A	0.9300	C14—C15	1.380 (5)
C4—C5	1.385 (4)	C14—H14A	0.9300
C4—C8	1.496 (4)	C15—H15A	0.9300
C5—C6	1.385 (4)	C16—H16A	0.9600
C6—C7	1.373 (5)	C16—H16B	0.9600
C6—H6A	0.9300	C16—H16C	0.9600
C9—N1—C10	122.3 (3)	N1—C8—H8B	109.4
C9—N1—C8	118.7 (3)	C4—C8—H8B	109.4

C10—N1—C8	118.3 (2)	H8A—C8—H8B	108.0
C9—N2—C5	116.2 (3)	N2—C9—N1	129.0 (3)
C2—C1—H1A	109.5	N2—C9—H9A	115.5
C2—C1—H1B	109.5	N1—C9—H9A	115.5
H1A—C1—H1B	109.5	C11—C10—C15	117.8 (3)
C2—C1—H1C	109.5	C11—C10—N1	120.5 (3)
H1A—C1—H1C	109.5	C15—C10—N1	121.8 (3)
H1B—C1—H1C	109.5	C12—C11—C10	121.0 (3)
C7—C2—C3	118.3 (4)	C12—C11—H11A	119.5
C7—C2—C1	121.4 (4)	C10—C11—H11A	119.5
C3—C2—C1	120.3 (4)	C11—C12—C13	121.7 (3)
C4—C3—C2	121.6 (3)	C11—C12—H12A	119.1
C4—C3—H3A	119.2	C13—C12—H12A	119.1
C2—C3—H3A	119.2	C14—C13—C12	116.6 (3)
C3—C4—C5	118.9 (3)	C14—C13—C16	122.8 (3)
C3—C4—C8	119.8 (3)	C12—C13—C16	120.5 (4)
C5—C4—C8	121.3 (3)	C13—C14—C15	123.0 (3)
C6—C5—C4	120.0 (3)	C13—C14—H14A	118.5
C6—C5—N2	118.6 (3)	C15—C14—H14A	118.5
C4—C5—N2	121.4 (3)	C14—C15—C10	119.8 (3)
C7—C6—C5	120.2 (4)	C14—C15—H15A	120.1
C7—C6—H6A	119.9	C10—C15—H15A	120.1
C5—C6—H6A	119.9	C13—C16—H16A	109.5
C6—C7—C2	120.9 (4)	C13—C16—H16B	109.5
C6—C7—H7A	119.5	H16A—C16—H16B	109.5
C2—C7—H7A	119.5	C13—C16—H16C	109.5
N1—C8—C4	111.4 (3)	H16A—C16—H16C	109.5
N1—C8—H8A	109.4	H16B—C16—H16C	109.5
C4—C8—H8A	109.4		
C7—C2—C3—C4	−1.5 (6)	C5—C4—C8—N1	−11.9 (4)
C1—C2—C3—C4	177.5 (3)	C5—N2—C9—N1	−1.1 (6)
C2—C3—C4—C5	1.6 (5)	C10—N1—C9—N2	178.4 (3)
C2—C3—C4—C8	−179.8 (3)	C8—N1—C9—N2	−11.0 (5)
C3—C4—C5—C6	−1.0 (5)	C9—N1—C10—C11	165.3 (3)
C8—C4—C5—C6	−179.6 (3)	C8—N1—C10—C11	−5.3 (4)
C3—C4—C5—N2	179.8 (3)	C9—N1—C10—C15	−15.7 (5)
C8—C4—C5—N2	1.2 (5)	C8—N1—C10—C15	173.6 (3)
C9—N2—C5—C6	−173.1 (3)	C15—C10—C11—C12	2.8 (5)
C9—N2—C5—C4	6.1 (5)	N1—C10—C11—C12	−178.2 (3)
C4—C5—C6—C7	0.4 (5)	C10—C11—C12—C13	−0.6 (5)
N2—C5—C6—C7	179.6 (3)	C11—C12—C13—C14	−0.9 (5)
C5—C6—C7—C2	−0.3 (6)	C11—C12—C13—C16	179.2 (3)
C3—C2—C7—C6	0.8 (6)	C12—C13—C14—C15	0.2 (5)
C1—C2—C7—C6	−178.2 (4)	C16—C13—C14—C15	−179.9 (3)
C9—N1—C8—C4	16.2 (4)	C13—C14—C15—C10	2.1 (6)
C10—N1—C8—C4	−172.8 (3)	C11—C10—C15—C14	−3.5 (5)
C3—C4—C8—N1	169.5 (3)	N1—C10—C15—C14	177.5 (3)

Fig. 1

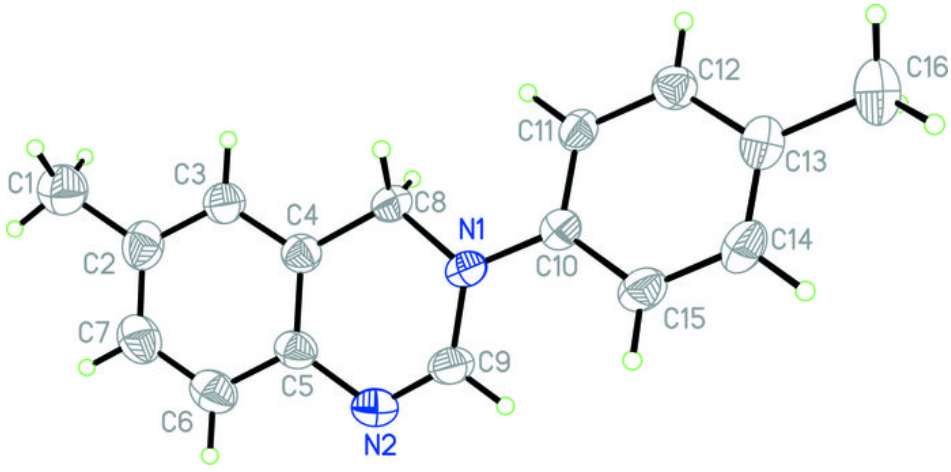

Fig. 2