Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Benzyl-3-phenylquinoxalin-2(1*H*)-one

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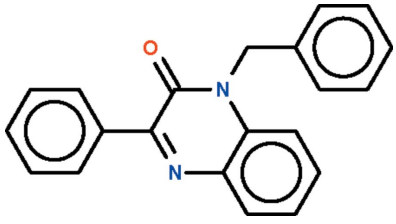
Received 29 September 2009; accepted 1 October 2009

Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.002 Å; R factor = 0.046; wR factor = 0.123; data-to-parameter ratio = 17.8.

The ten-membered fused ring system in the title compound, $C_{21}H_{16}N_2O_2$, is planar (r.m.s. deviation = 0.03 Å). The phenyl substituent is aligned at 15.1 (1)° with respect to the mean plane through this system, whereas the phenyl ring of the benzyl substitutent is aligned at 84.4 (1)°.

Related literature

For the crystal structure of the unsubstituted quinolixalin-2(1*H*)-one, see: Padmaja *et al.* (1987); Stępień *et al.* (1976).



Experimental

Crystal data

$C_{21}H_{16}N_2O$
M_r = 312.36
Triclinic, $P\overline{1}$
a = 5.4776 (2) Å
b = 12.7015 (3) Å
c = 12.7469 (4) Å
α = 62.260 (2)°
β = 89.963 (2)°
γ = 87.845 (2)°
V = 784.23 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 193 K
0.60 × 0.20 × 0.10 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: none
12094 measured reflections
3864 independent reflections
2613 reflections with $I > 2\sigma(I)$
R_{int} = 0.037

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.123
S = 1.04
3864 reflections
217 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank Université Mohammed V-Agdal and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2547).

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supporting information

Acta Cryst. (2009). E**65**, o2685 [https://doi.org/10.1107/S1600536809039944]

1-Benzyl-3-phenylquinoxalin-2(1*H*)-one

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S1. Experimental

To a solution of 3-phenylquinoxalin-2(*1H*)-one (1 g, 4.5 mmol) in *N*,*N*-dimethylformamide (20 ml) was added benzyl chloride (0.62 ml, 5.4 mmol), potassium carbonate (0.74 g; 5.4 mmol) and a catalytic quantity of tetra-n-butylammonium bromide. The mixture was stirred 24 h. The solution was filtered to remove the salts and the solvent then removed under reduced pressure. The residue was recrystallized from ethanol to afford yellow crystals in 85% yield.

S2. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2U_{eq}(C). The amino H-atom was located in a difference Fourier map and was refined with an N–H 0.88±0.01 Å restraint.

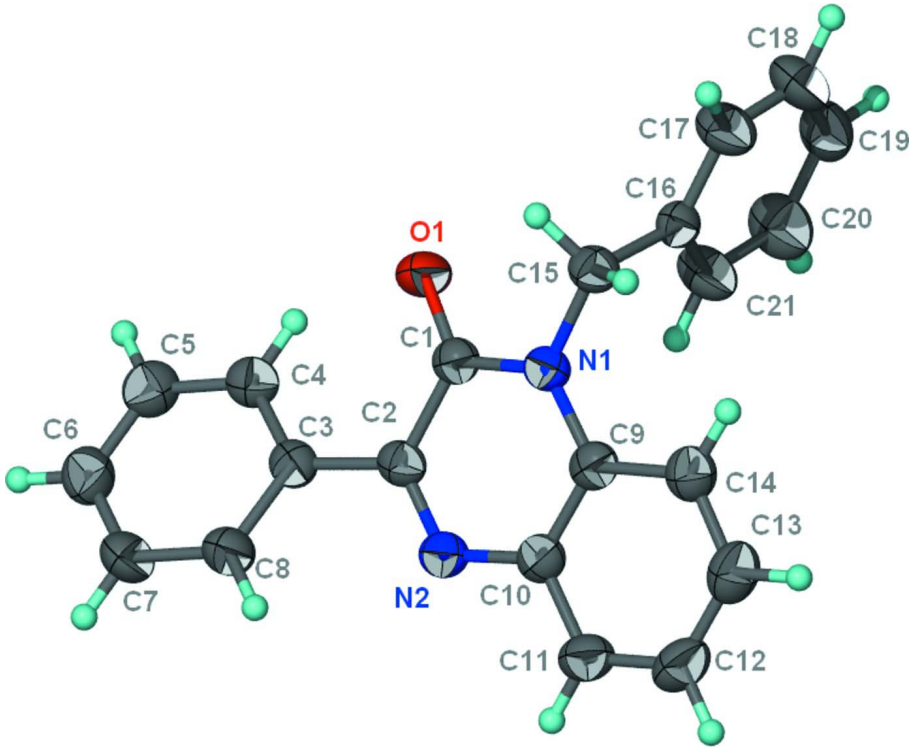

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{21}H_{16}N_2O$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

1-Benzyl-3-phenylquinoxalin-2(1*H*)-one

Crystal data

$C_{21}H_{16}N_2O$
$M_r = 312.36$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 5.4776$ (2) Å
$b = 12.7015$ (3) Å
$c = 12.7469$ (4) Å
$\alpha = 62.260$ (2)°
$\beta = 89.963$ (2)°
$\gamma = 87.845$ (2)°
$V = 784.23$ (4) Å^3
$Z = 2$
$F(000) = 328$
$D_x = 1.323$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2441 reflections
$\theta = 5.4$–$28.3°$
$\mu = 0.08$ mm^{-1}
$T = 193$ K
Plate, yellow
0.60 × 0.20 × 0.10 mm

Data collection

Bruker APEX2 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
12094 measured reflections
3864 independent reflections
2613 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 28.3°$, $\theta_{min} = 5.1°$
$h = -7 \rightarrow 7$
$k = -14 \rightarrow 16$
$l = 0 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.123$
$S = 1.04$
3864 reflections
217 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 0.0846P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8050 (2)	0.89874 (9)	0.53919 (8)	0.0380 (3)
N1	1.1349 (2)	0.77023 (10)	0.59168 (9)	0.0277 (3)
N2	0.9967 (2)	0.67563 (10)	0.82777 (10)	0.0305 (3)
C1	0.9290 (3)	0.81877 (12)	0.61835 (12)	0.0280 (3)
C2	0.8775 (3)	0.76874 (12)	0.74735 (11)	0.0276 (3)
C3	0.6910 (3)	0.82891 (12)	0.78827 (12)	0.0286 (3)
C4	0.4926 (3)	0.89908 (12)	0.71895 (13)	0.0319 (3)
H4	0.4715	0.9110	0.6402	0.038*
C5	0.3266 (3)	0.95134 (14)	0.76436 (14)	0.0381 (4)
H5	0.1920	0.9985	0.7164	0.046*
C6	0.3539 (3)	0.93598 (14)	0.87820 (14)	0.0407 (4)
H6	0.2388	0.9722	0.9086	0.049*
C7	0.5508 (3)	0.86731 (14)	0.94800 (13)	0.0412 (4)

H7	0.5715	0.8567	1.0264	0.049*
C8	0.7170 (3)	0.81428 (13)	0.90366 (13)	0.0361 (4)
H8	0.8510	0.7672	0.9522	0.043*
C9	1.2618 (3)	0.66951 (12)	0.67667 (12)	0.0289 (3)
C10	1.1849 (3)	0.62205 (12)	0.79476 (12)	0.0296 (3)
C11	1.3073 (3)	0.52005 (13)	0.88251 (13)	0.0360 (4)
H11	1.2555	0.4871	0.9623	0.043*
C12	1.5020 (3)	0.46731 (14)	0.85381 (14)	0.0408 (4)
H12	1.5861	0.3990	0.9138	0.049*
C13	1.5755 (3)	0.51431 (14)	0.73642 (15)	0.0408 (4)
H13	1.7093	0.4774	0.7169	0.049*
C14	1.4563 (3)	0.61377 (13)	0.64823 (13)	0.0349 (3)
H14	1.5065	0.6443	0.5684	0.042*
C15	1.2157 (3)	0.82914 (12)	0.46821 (12)	0.0303 (3)
H15A	1.3964	0.8232	0.4678	0.036*
H15B	1.1655	0.9147	0.4322	0.036*
C16	1.1145 (2)	0.77719 (12)	0.39268 (12)	0.0274 (3)
C17	1.1725 (3)	0.82793 (14)	0.27348 (13)	0.0417 (4)
H17	1.2813	0.8915	0.2418	0.050*
C18	1.0730 (3)	0.78651 (16)	0.20034 (14)	0.0483 (4)
H18	1.1141	0.8222	0.1189	0.058*
C19	0.9165 (3)	0.69502 (15)	0.24384 (15)	0.0445 (4)
H19	0.8474	0.6678	0.1929	0.053*
C20	0.8597 (3)	0.64252 (16)	0.36247 (15)	0.0491 (4)
H20	0.7524	0.5783	0.3938	0.059*
C21	0.9601 (3)	0.68376 (14)	0.43620 (13)	0.0401 (4)
H21	0.9213	0.6467	0.5179	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0422 (6)	0.0378 (6)	0.0273 (5)	0.0079 (5)	−0.0037 (5)	−0.0103 (5)
N1	0.0307 (6)	0.0279 (6)	0.0243 (6)	−0.0009 (5)	−0.0005 (5)	−0.0120 (5)
N2	0.0353 (7)	0.0283 (6)	0.0267 (6)	−0.0012 (5)	−0.0012 (5)	−0.0119 (5)
C1	0.0310 (8)	0.0261 (7)	0.0278 (7)	−0.0022 (6)	−0.0023 (6)	−0.0131 (6)
C2	0.0300 (7)	0.0283 (7)	0.0256 (7)	−0.0054 (6)	−0.0005 (6)	−0.0131 (6)
C3	0.0298 (7)	0.0278 (7)	0.0287 (7)	−0.0050 (6)	0.0029 (6)	−0.0132 (6)
C4	0.0305 (8)	0.0334 (8)	0.0321 (7)	−0.0040 (6)	−0.0014 (6)	−0.0153 (6)
C5	0.0300 (8)	0.0397 (8)	0.0421 (9)	−0.0001 (6)	0.0016 (7)	−0.0170 (7)
C6	0.0407 (9)	0.0398 (9)	0.0409 (9)	−0.0013 (7)	0.0113 (7)	−0.0184 (7)
C7	0.0491 (10)	0.0446 (9)	0.0289 (7)	0.0022 (8)	0.0048 (7)	−0.0167 (7)
C8	0.0390 (9)	0.0388 (8)	0.0284 (7)	0.0037 (7)	−0.0009 (6)	−0.0143 (6)
C9	0.0302 (8)	0.0269 (7)	0.0311 (7)	−0.0025 (6)	−0.0047 (6)	−0.0149 (6)
C10	0.0309 (8)	0.0293 (7)	0.0303 (7)	−0.0010 (6)	−0.0041 (6)	−0.0153 (6)
C11	0.0417 (9)	0.0320 (8)	0.0306 (7)	0.0006 (7)	−0.0060 (7)	−0.0115 (6)
C12	0.0408 (9)	0.0324 (8)	0.0447 (9)	0.0068 (7)	−0.0106 (7)	−0.0147 (7)
C13	0.0341 (9)	0.0401 (9)	0.0518 (10)	0.0053 (7)	−0.0034 (7)	−0.0247 (8)
C14	0.0324 (8)	0.0370 (8)	0.0374 (8)	−0.0007 (6)	0.0013 (6)	−0.0192 (7)

C15	0.0319 (8)	0.0298 (7)	0.0275 (7)	−0.0049 (6)	0.0034 (6)	−0.0116 (6)
C16	0.0267 (7)	0.0283 (7)	0.0276 (7)	0.0025 (6)	0.0000 (6)	−0.0136 (6)
C17	0.0480 (10)	0.0441 (9)	0.0312 (8)	−0.0106 (8)	0.0083 (7)	−0.0155 (7)
C18	0.0596 (11)	0.0584 (11)	0.0299 (8)	−0.0017 (9)	0.0045 (8)	−0.0231 (8)
C19	0.0486 (10)	0.0516 (10)	0.0437 (9)	0.0048 (8)	−0.0100 (8)	−0.0316 (8)
C20	0.0533 (11)	0.0530 (10)	0.0497 (10)	−0.0177 (8)	0.0027 (8)	−0.0300 (9)
C21	0.0445 (9)	0.0464 (9)	0.0320 (8)	−0.0139 (7)	0.0068 (7)	−0.0197 (7)

Geometric parameters (Å, º)

O1—C1	1.2274 (15)	C11—C12	1.376 (2)
N1—C1	1.3820 (18)	C11—H11	0.9500
N1—C9	1.3918 (17)	C12—C13	1.394 (2)
N1—C15	1.4698 (16)	C12—H12	0.9500
N2—C2	1.3000 (17)	C13—C14	1.379 (2)
N2—C10	1.3843 (18)	C13—H13	0.9500
C1—C2	1.4925 (18)	C14—H14	0.9500
C2—C3	1.4872 (19)	C15—C16	1.5132 (18)
C3—C4	1.3971 (19)	C15—H15A	0.9900
C3—C8	1.4008 (19)	C15—H15B	0.9900
C4—C5	1.383 (2)	C16—C21	1.376 (2)
C4—H4	0.9500	C16—C17	1.3887 (19)
C5—C6	1.379 (2)	C17—C18	1.386 (2)
C5—H5	0.9500	C17—H17	0.9500
C6—C7	1.387 (2)	C18—C19	1.366 (3)
C6—H6	0.9500	C18—H18	0.9500
C7—C8	1.382 (2)	C19—C20	1.380 (2)
C7—H7	0.9500	C19—H19	0.9500
C8—H8	0.9500	C20—C21	1.393 (2)
C9—C14	1.396 (2)	C20—H20	0.9500
C9—C10	1.4071 (19)	C21—H21	0.9500
C10—C11	1.4021 (19)		
C1—N1—C9	122.23 (11)	C12—C11—H11	119.8
C1—N1—C15	117.13 (11)	C10—C11—H11	119.8
C9—N1—C15	120.63 (11)	C11—C12—C13	119.83 (14)
C2—N2—C10	119.69 (12)	C11—C12—H12	120.1
O1—C1—N1	120.56 (12)	C13—C12—H12	120.1
O1—C1—C2	124.30 (13)	C14—C13—C12	120.87 (15)
N1—C1—C2	115.13 (11)	C14—C13—H13	119.6
N2—C2—C3	117.57 (12)	C12—C13—H13	119.6
N2—C2—C1	122.49 (12)	C13—C14—C9	119.81 (14)
C3—C2—C1	119.89 (11)	C13—C14—H14	120.1
C4—C3—C8	118.12 (13)	C9—C14—H14	120.1
C4—C3—C2	124.19 (12)	N1—C15—C16	113.80 (11)
C8—C3—C2	117.69 (12)	N1—C15—H15A	108.8
C5—C4—C3	120.39 (13)	C16—C15—H15A	108.8
C5—C4—H4	119.8	N1—C15—H15B	108.8

C3—C4—H4	119.8	C16—C15—H15B	108.8
C6—C5—C4	120.92 (14)	H15A—C15—H15B	107.7
C6—C5—H5	119.5	C21—C16—C17	118.26 (13)
C4—C5—H5	119.5	C21—C16—C15	122.73 (12)
C5—C6—C7	119.48 (14)	C17—C16—C15	118.99 (13)
C5—C6—H6	120.3	C18—C17—C16	120.52 (15)
C7—C6—H6	120.3	C18—C17—H17	119.7
C8—C7—C6	120.05 (14)	C16—C17—H17	119.7
C8—C7—H7	120.0	C19—C18—C17	120.85 (15)
C6—C7—H7	120.0	C19—C18—H18	119.6
C7—C8—C3	121.03 (14)	C17—C18—H18	119.6
C7—C8—H8	119.5	C18—C19—C20	119.34 (15)
C3—C8—H8	119.5	C18—C19—H19	120.3
N1—C9—C14	122.46 (13)	C20—C19—H19	120.3
N1—C9—C10	117.81 (12)	C19—C20—C21	119.91 (16)
C14—C9—C10	119.71 (13)	C19—C20—H20	120.0
N2—C10—C11	118.79 (13)	C21—C20—H20	120.0
N2—C10—C9	121.84 (12)	C16—C21—C20	121.11 (14)
C11—C10—C9	119.33 (13)	C16—C21—H21	119.4
C12—C11—C10	120.43 (14)	C20—C21—H21	119.4

C9—N1—C1—O1	−171.38 (12)	C2—N2—C10—C11	−178.50 (12)
C15—N1—C1—O1	8.22 (18)	C2—N2—C10—C9	3.8 (2)
C9—N1—C1—C2	9.96 (18)	N1—C9—C10—N2	−2.82 (19)
C15—N1—C1—C2	−170.44 (11)	C14—C9—C10—N2	178.51 (12)
C10—N2—C2—C3	−175.06 (12)	N1—C9—C10—C11	179.47 (12)
C10—N2—C2—C1	2.35 (19)	C14—C9—C10—C11	0.8 (2)
O1—C1—C2—N2	172.36 (13)	N2—C10—C11—C12	−177.24 (13)
N1—C1—C2—N2	−9.05 (18)	C9—C10—C11—C12	0.5 (2)
O1—C1—C2—C3	−10.3 (2)	C10—C11—C12—C13	−1.1 (2)
N1—C1—C2—C3	168.30 (11)	C11—C12—C13—C14	0.4 (2)
N2—C2—C3—C4	−155.97 (13)	C12—C13—C14—C9	1.0 (2)
C1—C2—C3—C4	26.6 (2)	N1—C9—C14—C13	179.85 (13)
N2—C2—C3—C8	24.20 (19)	C10—C9—C14—C13	−1.5 (2)
C1—C2—C3—C8	−153.28 (13)	C1—N1—C15—C16	−92.98 (14)
C8—C3—C4—C5	−0.5 (2)	C9—N1—C15—C16	86.63 (15)
C2—C3—C4—C5	179.64 (13)	N1—C15—C16—C21	0.29 (19)
C3—C4—C5—C6	0.4 (2)	N1—C15—C16—C17	178.13 (13)
C4—C5—C6—C7	0.1 (2)	C21—C16—C17—C18	1.2 (2)
C5—C6—C7—C8	−0.4 (2)	C15—C16—C17—C18	−176.71 (14)
C6—C7—C8—C3	0.2 (2)	C16—C17—C18—C19	−0.1 (3)
C4—C3—C8—C7	0.2 (2)	C17—C18—C19—C20	−0.8 (3)
C2—C3—C8—C7	−179.92 (14)	C18—C19—C20—C21	0.6 (3)
C1—N1—C9—C14	174.04 (12)	C17—C16—C21—C20	−1.4 (2)
C15—N1—C9—C14	−5.54 (19)	C15—C16—C21—C20	176.43 (14)
C1—N1—C9—C10	−4.59 (18)	C19—C20—C21—C16	0.5 (3)
C15—N1—C9—C10	175.83 (12)		