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1-Phenyl-3*H*-2,3-benzodiazepin-4(5*H*)-one

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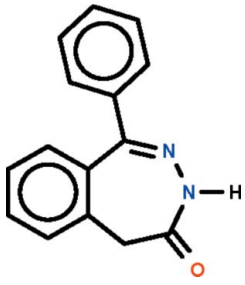
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.040; wR factor = 0.115; data-to-parameter ratio = 9.8.

The seven-membered ring in the title compound, $C_{15}H_{12}N_2O$, adopts a boat-shaped conformation (with the methylene C atom as the prow and the double-bond C=N pair of atoms as the stern). In the crystal, adjacent molecules are linked by an N—H···O hydrogen bond to generate helical chains running along the *a* axis of the orthorhombic unit cell.

Related literature

For the synthesis and pharmacological properties of the title compound, see: Flammang & Wermuth (1976); Wermuth & Flammang (1971). For related structures, see: Bruno *et al.* (2001, 2003).



Experimental

Crystal data

$C_{15}H_{12}N_2O$
M_r = 236.27
Orthorhombic, $P2_12_12_1$
a = 5.4718 (1) Å
b = 8.4020 (1) Å
c = 26.3250 (5) Å
V = 1210.27 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 K
0.23 × 0.20 × 0.17 mm

Data collection

Bruker APEX DUO CCD diffractometer
9472 measured reflections
2063 independent reflections
1899 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.115
S = 1.04
2063 reflections
211 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O1^{i}	0.90 (3)	1.92 (3)	2.812 (2)	176 (2)

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, -z$.

Data collection: *APEX2* (Bruker, 2010); cell refinement: *SAINT* (Bruker, 2010); 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, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2221).

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supporting information

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1-Phenyl-3*H*-2,3-benzodiazepin-4(5*H*)-one

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S1. Comment

The benzodiazepinone homolog, $C_{15}H_{12}N_2O$ (Scheme I), is a pharmacological compound exhibiting tranquilizer activity; its crystal structure has not previously been reported. When the benzene ring that is fused with the seven-membered ring carries a dioxolo substituent, the compound exists as a centrosymmetric dimer that is held together by an N—H···N hydrogen bond [3.030 (3) Å] (Bruno *et al.*, 2003). In contrast, with a pair of methoxy substituents, the compound is also a centrosymmetric dimer but the two halves are held together by an N—H···O hydrogen bond [2.876 (2) Å] (Bruno *et al.*, 2001).

The seven-membered ring in $C_{15}H_{12}N_2O$ adopts a boat-shaped conformation (Fig. 1). Adjacent molecules are linked by an N—H···O hydrogen bond (Table 1) to generate one-dimensional helical chains running along the *a*-axis of the orthorhombic unit cell (Fig. 2).

S2. Experimental

Ethoxycarbonylmethyl-2-benzophenone (1.34 g, 5 mmol) was heated with hydrazine hydrate (0.50 g, 10 mmol) in ethanol (30 ml) for 3 hours with the progress of the reaction monitored by thin layer chromatography. The solvent was removed and the white powder was recrystallized from ethanol to affford colorless crystals. The procedure was that reported in the literature (Flammang & Wermuth, 1976; Wermuth & Flammang, 1971).

S3. Refinement

Hydrogen atoms were freely refined. The (0 0 2) reflection was omitted owing to bad disagreement. In the absence of heavy atoms, 1461 Friedel pairs were merged.

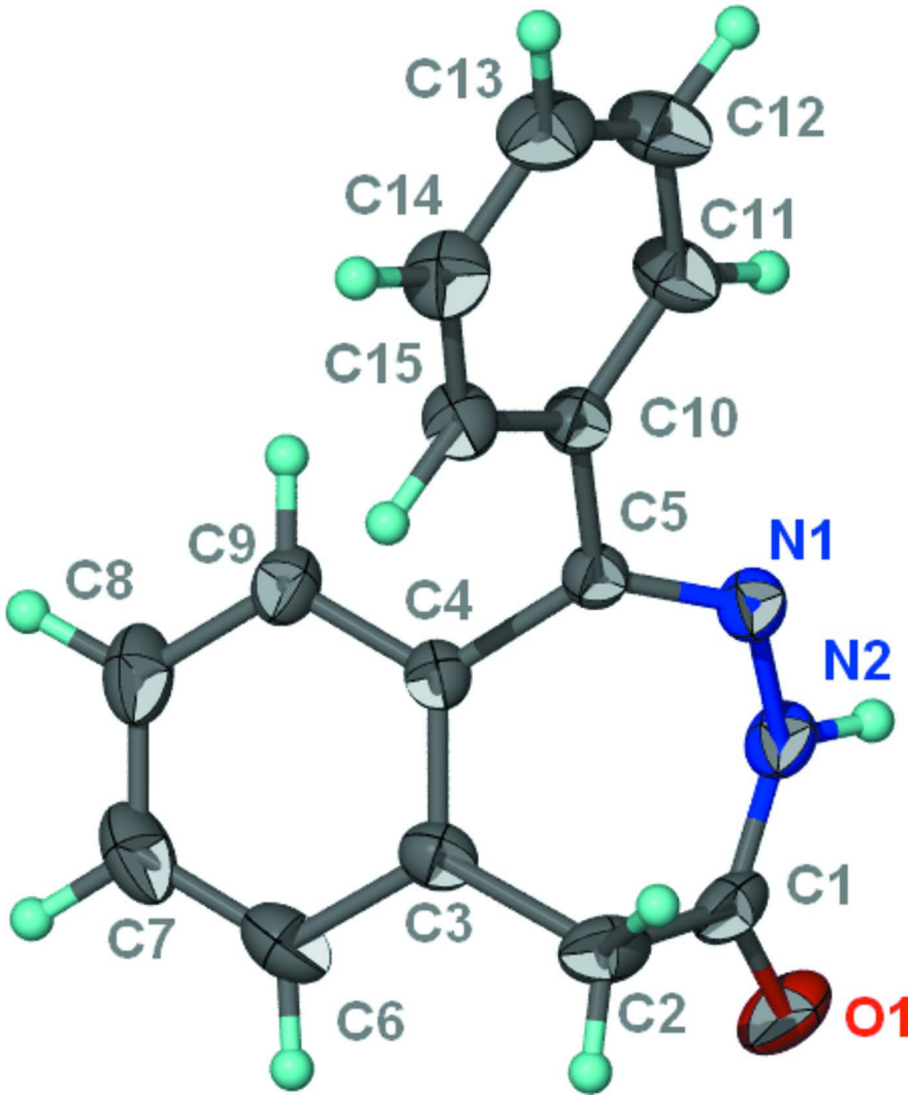

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{15}H_{12}N_2O_2$ at the 50% probability level.

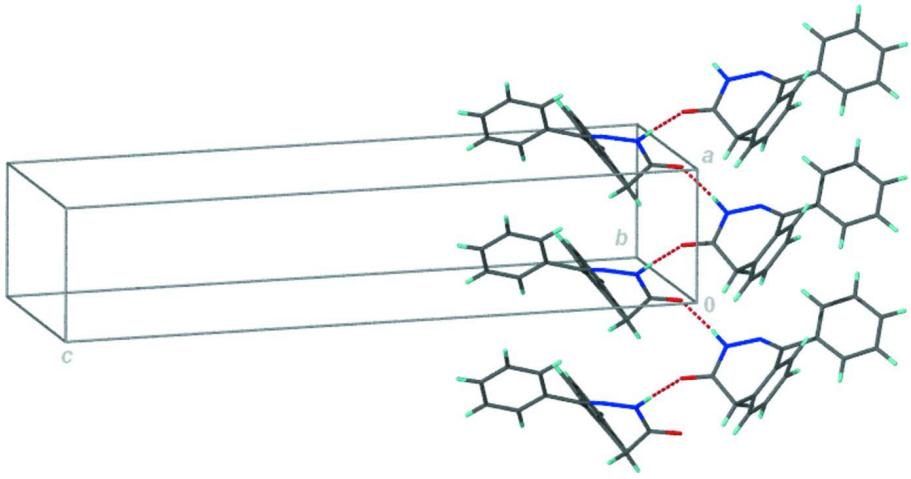

Figure 2

Hydrogen-bonded chain motif.

1-Phenyl-3*H*-2,3-benzodiazepin-4(5*H*)-one

Crystal data

$C_{15}H_{12}N_2O$
$M_r = 236.27$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 5.4718$ (1) Å
$b = 8.4020$ (1) Å
$c = 26.3250$ (5) Å
$V = 1210.27$ (4) Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.297$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4920 reflections
$\theta = 2.9$–$32.7°$
$\mu = 0.08$ mm^{-1}
$T = 293$ K
Prism, colorless
0.23 × 0.20 × 0.17 mm

Data collection

Bruker APEX DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
9472 measured reflections
2063 independent reflections
1899 reflections with $I > 2\sigma(I)$
$R_{int} = 0.021$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.9°$
$h = -7 \rightarrow 7$
$k = -10 \rightarrow 11$
$l = -37 \rightarrow 35$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.115$
$S = 1.04$
2063 reflections
211 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
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0814P)^2 + 0.0803P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	−0.1095 (3)	0.36819 (18)	−0.01027 (5)	0.0604 (4)
N1	0.1515 (3)	0.37477 (15)	0.11324 (4)	0.0380 (3)
N2	0.1083 (3)	0.36162 (16)	0.06118 (5)	0.0413 (3)
C1	−0.0928 (3)	0.40531 (19)	0.03479 (6)	0.0424 (3)
C2	−0.2805 (3)	0.5014 (2)	0.06309 (7)	0.0477 (4)
C3	−0.1668 (3)	0.6578 (2)	0.07707 (5)	0.0382 (3)
C4	0.0289 (3)	0.65874 (16)	0.11127 (5)	0.0329 (3)
C5	0.1167 (3)	0.51028 (16)	0.13530 (5)	0.0319 (3)
C6	−0.2431 (4)	0.8013 (3)	0.05550 (7)	0.0520 (4)
C7	−0.1259 (5)	0.9415 (2)	0.06675 (7)	0.0582 (5)
C8	0.0708 (5)	0.9426 (2)	0.09960 (7)	0.0545 (5)
C9	0.1462 (4)	0.80259 (19)	0.12240 (6)	0.0420 (4)
C10	0.1850 (3)	0.51417 (17)	0.19011 (5)	0.0336 (3)
C11	0.3855 (3)	0.4275 (2)	0.20722 (6)	0.0468 (4)
C12	0.4501 (4)	0.4305 (3)	0.25822 (7)	0.0570 (5)
C13	0.3130 (4)	0.5173 (3)	0.29244 (6)	0.0555 (5)
C14	0.1132 (4)	0.6027 (2)	0.27610 (6)	0.0514 (4)
C15	0.0503 (3)	0.6029 (2)	0.22465 (6)	0.0419 (3)
H2	0.201 (5)	0.287 (3)	0.0465 (9)	0.057 (6)*
H21	−0.325 (5)	0.439 (3)	0.0955 (8)	0.052 (6)*
H22	−0.422 (6)	0.513 (3)	0.0425 (10)	0.074 (8)*
H6	−0.385 (5)	0.794 (3)	0.0333 (10)	0.072 (8)*
H7	−0.183 (6)	1.042 (4)	0.0503 (10)	0.082 (9)*
H8	0.146 (5)	1.046 (3)	0.1093 (9)	0.063 (7)*
H9	0.288 (4)	0.803 (3)	0.1463 (8)	0.051 (5)*
H11	0.486 (6)	0.358 (3)	0.1827 (9)	0.067 (7)*
H12	0.595 (5)	0.365 (3)	0.2686 (9)	0.057 (6)*
H13	0.349 (6)	0.514 (4)	0.3290 (10)	0.087 (9)*
H14	0.015 (6)	0.672 (3)	0.2998 (9)	0.065 (7)*
H15	−0.088 (5)	0.666 (3)	0.2125 (8)	0.059 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0822 (9)	0.0608 (8)	0.0383 (6)	−0.0207 (8)	−0.0137 (6)	−0.0071 (5)
N1	0.0475 (7)	0.0350 (6)	0.0315 (5)	0.0012 (6)	−0.0012 (5)	−0.0018 (4)
N2	0.0526 (8)	0.0387 (6)	0.0328 (6)	−0.0001 (6)	−0.0006 (5)	−0.0077 (5)
C1	0.0505 (8)	0.0393 (7)	0.0374 (7)	−0.0179 (7)	−0.0053 (6)	−0.0008 (5)
C2	0.0350 (7)	0.0592 (10)	0.0490 (8)	−0.0102 (7)	−0.0059 (6)	0.0025 (8)
C3	0.0339 (7)	0.0451 (7)	0.0358 (6)	0.0030 (6)	0.0004 (5)	0.0026 (5)
C4	0.0374 (6)	0.0324 (6)	0.0289 (5)	0.0017 (6)	0.0023 (5)	0.0007 (5)
C5	0.0341 (6)	0.0320 (6)	0.0296 (5)	−0.0008 (5)	−0.0007 (5)	0.0005 (5)
C6	0.0492 (10)	0.0595 (10)	0.0474 (8)	0.0156 (9)	−0.0022 (8)	0.0102 (8)
C7	0.0819 (14)	0.0437 (9)	0.0490 (9)	0.0177 (10)	0.0068 (10)	0.0132 (7)
C8	0.0848 (14)	0.0341 (7)	0.0446 (8)	−0.0021 (9)	0.0065 (9)	0.0037 (6)

C9	0.0577 (10)	0.0346 (6)	0.0339 (6)	−0.0051 (7)	−0.0014 (7)	−0.0005 (5)
C10	0.0381 (7)	0.0336 (6)	0.0292 (5)	−0.0008 (6)	−0.0012 (5)	0.0015 (5)
C11	0.0477 (9)	0.0566 (9)	0.0362 (7)	0.0121 (8)	−0.0011 (6)	0.0046 (6)
C12	0.0551 (10)	0.0753 (13)	0.0408 (8)	0.0099 (11)	−0.0076 (7)	0.0116 (8)
C13	0.0683 (12)	0.0683 (11)	0.0300 (6)	−0.0056 (11)	−0.0064 (7)	0.0053 (7)
C14	0.0671 (11)	0.0554 (9)	0.0318 (7)	0.0003 (9)	0.0054 (7)	−0.0036 (7)
C15	0.0489 (8)	0.0424 (8)	0.0345 (6)	0.0050 (7)	0.0021 (6)	−0.0002 (6)

Geometric parameters (Å, º)

O1—C1	1.2301 (19)	C7—C8	1.380 (3)
N1—C5	1.2922 (18)	C7—H7	1.00 (3)
N1—N2	1.3951 (16)	C8—C9	1.383 (2)
N2—C1	1.352 (2)	C8—H8	1.00 (3)
N2—H2	0.90 (3)	C9—H9	1.00 (2)
C1—C2	1.504 (3)	C10—C15	1.388 (2)
C2—C3	1.500 (3)	C10—C11	1.392 (2)
C2—H21	1.03 (2)	C11—C12	1.389 (2)
C2—H22	0.95 (3)	C11—H11	1.03 (3)
C3—C6	1.397 (2)	C12—C13	1.381 (3)
C3—C4	1.399 (2)	C12—H12	1.00 (3)
C4—C9	1.400 (2)	C13—C14	1.377 (3)
C4—C5	1.4790 (19)	C13—H13	0.98 (3)
C5—C10	1.4907 (17)	C14—C15	1.398 (2)
C6—C7	1.374 (3)	C14—H14	1.01 (3)
C6—H6	0.97 (3)	C15—H15	0.98 (3)
C5—N1—N2	119.10 (12)	C6—C7—H7	119.1 (18)
C1—N2—N1	128.39 (15)	C8—C7—H7	120.6 (18)
C1—N2—H2	115.5 (15)	C7—C8—C9	119.94 (18)
N1—N2—H2	112.5 (15)	C7—C8—H8	119.2 (16)
O1—C1—N2	119.15 (18)	C9—C8—H8	120.6 (16)
O1—C1—C2	124.27 (17)	C8—C9—C4	120.42 (16)
N2—C1—C2	116.56 (14)	C8—C9—H9	120.3 (14)
C3—C2—C1	107.98 (13)	C4—C9—H9	119.3 (14)
C3—C2—H21	109.8 (13)	C15—C10—C11	119.20 (14)
C1—C2—H21	107.4 (13)	C15—C10—C5	120.85 (13)
C3—C2—H22	112.8 (17)	C11—C10—C5	119.95 (13)
C1—C2—H22	109.2 (17)	C12—C11—C10	120.27 (16)
H21—C2—H22	109 (2)	C12—C11—H11	118.7 (15)
C6—C3—C4	119.03 (16)	C10—C11—H11	121.0 (15)
C6—C3—C2	122.19 (15)	C13—C12—C11	120.13 (18)
C4—C3—C2	118.73 (14)	C13—C12—H12	122.8 (13)
C3—C4—C9	119.40 (14)	C11—C12—H12	117.0 (14)
C3—C4—C5	121.27 (13)	C14—C13—C12	120.21 (15)
C9—C4—C5	119.32 (13)	C14—C13—H13	118.6 (19)
N1—C5—C4	126.78 (12)	C12—C13—H13	121.1 (19)
N1—C5—C10	114.67 (12)	C13—C14—C15	119.92 (17)

C4—C5—C10	118.49 (12)	C13—C14—H14	122.0 (15)
C7—C6—C3	120.88 (17)	C15—C14—H14	117.9 (15)
C7—C6—H6	123.6 (17)	C10—C15—C14	120.24 (16)
C3—C6—H6	115.5 (17)	C10—C15—H15	119.1 (13)
C6—C7—C8	120.30 (16)	C14—C15—H15	120.6 (13)
C5—N1—N2—C1	−51.1 (2)	C2—C3—C6—C7	−176.05 (19)
N1—N2—C1—O1	−171.86 (15)	C3—C6—C7—C8	0.2 (3)
N1—N2—C1—C2	9.7 (2)	C6—C7—C8—C9	−1.7 (3)
O1—C1—C2—C3	−113.71 (17)	C7—C8—C9—C4	1.8 (3)
N2—C1—C2—C3	64.68 (19)	C3—C4—C9—C8	−0.4 (2)
C1—C2—C3—C6	112.02 (18)	C5—C4—C9—C8	178.66 (15)
C1—C2—C3—C4	−65.26 (18)	N1—C5—C10—C15	−144.11 (15)
C6—C3—C4—C9	−1.1 (2)	C4—C5—C10—C15	38.6 (2)
C2—C3—C4—C9	176.25 (15)	N1—C5—C10—C11	35.6 (2)
C6—C3—C4—C5	179.85 (15)	C4—C5—C10—C11	−141.71 (16)
C2—C3—C4—C5	−2.8 (2)	C15—C10—C11—C12	−0.2 (3)
N2—N1—C5—C4	1.2 (2)	C5—C10—C11—C12	−179.95 (18)
N2—N1—C5—C10	−175.89 (13)	C10—C11—C12—C13	1.1 (3)
C3—C4—C5—N1	44.0 (2)	C11—C12—C13—C14	−0.7 (3)
C9—C4—C5—N1	−135.03 (17)	C12—C13—C14—C15	−0.6 (3)
C3—C4—C5—C10	−139.02 (14)	C11—C10—C15—C14	−1.1 (3)
C9—C4—C5—C10	41.9 (2)	C5—C10—C15—C14	178.62 (16)
C4—C3—C6—C7	1.2 (3)	C13—C14—C15—C10	1.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.90 (3)	1.92 (3)	2.812 (2)	176 (2)

Symmetry code: (i) *x*+1/2, −*y*+1/2, −*z*.