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3-Allyl-1,5-dibenzyl-1,5-benzodiazepine-2,4-dione

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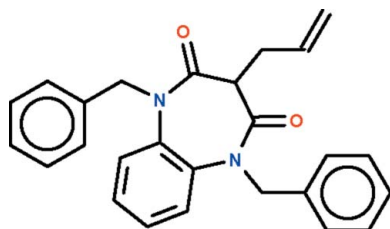
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Key indicators: single-crystal X-ray study; $T = 193$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.043; wR factor = 0.117; data-to-parameter ratio = 17.8.

The title compound, $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_2$, features a benzene ring fused with a seven-membered diazepine ring; the latter ring adopts a boat conformation (with the allyldimethylamino-methyl-bearing C atom as the prow and the fused-ring C atoms as the stern).

Related literature

For the crystal structure of benzodiazepin-2,4-dione, see: Négrier *et al.* (2006).



Experimental

Crystal data

$\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_2$
 $M_r = 396.47$
 Monoclinic, $P2_1/c$
 $a = 9.2603$ (4) Å
 $b = 14.0037$ (6) Å
 $c = 16.2249$ (7) Å
 $\beta = 91.996$ (1)°
 $V = 2102.7$ (2) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 193$ K
 $0.40 \times 0.40 \times 0.07$ mm

Data collection

Bruker APEXII diffractometer
 Absorption correction: none
 27620 measured reflections
 4820 independent reflections
 2934 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.117$
 $S = 1.00$
 4820 reflections
 271 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.21$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.18$ 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).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ2680).

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supplementary materials

Acta Cryst. (2009). E65, o3150 [doi:10.1107/S160053680904851X]

3-Allyl-1,5-dibenzyl-1,5-benzodiazepine-2,4-dione

H. Jabli, Y. Kandri Rodi, N. Saffon, E. M. Essassi and S. W. Ng

Experimental

To a solution of the potassium *t*-butoxide (0.24 g, 2.13 mmol) in THF (15 ml) was added 1,5-dibenzyl-1,5-benzodiazepine-2,4-dione (0.50 g, 1.40 mmol) and allyl bromide (0.20 ml, 1.88 mmol). Stirring was continued for 24 h. The reaction was monitored by thin layer chromatography. The mixture was filtered and the solution evaporated to give colorless crystals.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 1.00 Å) and were included in the refinement in the riding model approximation, with $U(\text{H})$ set to $1.2U(\text{C})$.

Figures

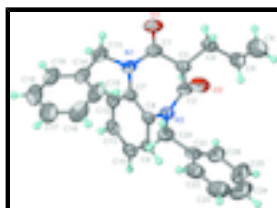


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

3-Allyl-1,5-dibenzyl-1,5-benzodiazepine-2,4-dione

Crystal data

$\text{C}_{26}\text{H}_{24}\text{N}_2\text{O}_2$	$F_{000} = 840$
$M_r = 396.47$	$D_x = 1.252 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 4269 reflections
$a = 9.2603 (4) \text{ \AA}$	$\theta = 2.5\text{--}25.0^\circ$
$b = 14.0037 (6) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 16.2249 (7) \text{ \AA}$	$T = 193 \text{ K}$
$\beta = 91.996 (1)^\circ$	Plate, colorless
$V = 2102.7 (2) \text{ \AA}^3$	$0.40 \times 0.40 \times 0.07 \text{ mm}$
$Z = 4$	

Data collection

Bruker APEXII diffractometer	2934 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{\text{int}} = 0.050$

supplementary materials

Monochromator: graphite $\theta_{\max} = 27.5^\circ$
 $T = 193$ K $\theta_{\min} = 1.9^\circ$
 φ and ω scans $h = -11 \rightarrow 12$
Absorption correction: None $k = -18 \rightarrow 18$
27620 measured reflections $l = -21 \rightarrow 16$
4820 independent reflections

Refinement

Refinement on F^2 Secondary atom site location: difference Fourier map
Least-squares matrix: full Hydrogen site location: inferred from neighbouring sites
 $R[F^2 > 2\sigma(F^2)] = 0.043$ H-atom parameters constrained
 $wR(F^2) = 0.117$ $w = 1/[\sigma^2(F_o^2) + (0.0487P)^2 + 0.414P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $S = 1.00$ $(\Delta/\sigma)_{\max} = 0.001$
4820 reflections $\Delta\rho_{\max} = 0.21 \text{ e } \text{\AA}^{-3}$
271 parameters $\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods Extinction correction: none

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.49018 (14)	0.26136 (9)	0.33899 (7)	0.0470 (3)
O2	0.33507 (16)	0.40157 (8)	0.16934 (7)	0.0498 (4)
N1	0.50477 (15)	0.15481 (9)	0.23332 (8)	0.0330 (3)
N2	0.37563 (15)	0.26484 (9)	0.09974 (7)	0.0320 (3)
C1	0.43555 (19)	0.22301 (11)	0.27747 (10)	0.0348 (4)
C2	0.33193 (19)	0.31439 (11)	0.16711 (9)	0.0350 (4)
C3	0.28998 (18)	0.25375 (11)	0.24091 (9)	0.0336 (4)
H3	0.2349	0.1963	0.2210	0.040*
C4	0.2006 (2)	0.30886 (12)	0.30184 (10)	0.0409 (4)
H4A	0.1979	0.2725	0.3541	0.049*
H4B	0.2479	0.3709	0.3139	0.049*
C5	0.0492 (2)	0.32639 (13)	0.27024 (11)	0.0485 (5)
H5	0.0365	0.3419	0.2135	0.058*
C6	-0.0667 (3)	0.32235 (16)	0.31310 (14)	0.0658 (6)
H6A	-0.0595	0.3071	0.3701	0.079*
H6B	-0.1585	0.3347	0.2874	0.079*
C7	0.43855 (17)	0.10939 (11)	0.16252 (9)	0.0294 (3)
C8	0.37894 (16)	0.16300 (10)	0.09694 (9)	0.0285 (3)
C9	0.32362 (17)	0.11561 (12)	0.02736 (9)	0.0332 (4)
H9	0.2852	0.1515	-0.0180	0.040*
C10	0.32381 (18)	0.01744 (12)	0.02331 (10)	0.0371 (4)
H10	0.2853	-0.0140	-0.0245	0.045*
C11	0.38017 (18)	-0.03554 (12)	0.08892 (10)	0.0361 (4)
H11	0.3788	-0.1033	0.0866	0.043*

C12	0.43813 (17)	0.01011 (11)	0.15748 (10)	0.0331 (4)
H12	0.4784	-0.0265	0.2019	0.040*
C13	0.65246 (19)	0.12564 (13)	0.25940 (10)	0.0407 (4)
H13A	0.6512	0.0580	0.2772	0.049*
H13B	0.6853	0.1648	0.3073	0.049*
C14	0.75779 (18)	0.13696 (12)	0.19117 (10)	0.0382 (4)
C15	0.7462 (2)	0.21035 (14)	0.13427 (12)	0.0483 (5)
H15	0.6699	0.2554	0.1376	0.058*
C16	0.8450 (2)	0.21874 (16)	0.07231 (13)	0.0603 (6)
H16	0.8353	0.2689	0.0331	0.072*
C17	0.9570 (2)	0.15453 (16)	0.06759 (14)	0.0606 (6)
H17	1.0243	0.1602	0.0250	0.073*
C18	0.9714 (2)	0.08237 (15)	0.12436 (14)	0.0564 (5)
H18	1.0498	0.0389	0.1218	0.068*
C19	0.8714 (2)	0.07300 (13)	0.18536 (12)	0.0459 (5)
H19	0.8808	0.0220	0.2238	0.055*
C20	0.4289 (2)	0.32016 (12)	0.02996 (10)	0.0380 (4)
H20A	0.4780	0.2757	-0.0073	0.046*
H20B	0.5023	0.3659	0.0516	0.046*
C21	0.3168 (2)	0.37497 (12)	-0.02019 (9)	0.0385 (4)
C22	0.3657 (3)	0.43780 (13)	-0.07970 (11)	0.0553 (5)
H22	0.4664	0.4466	-0.0858	0.066*
C23	0.2682 (4)	0.48731 (17)	-0.12977 (13)	0.0764 (8)
H23	0.3021	0.5301	-0.1702	0.092*
C24	0.1224 (4)	0.47491 (18)	-0.12138 (15)	0.0839 (9)
H24	0.0558	0.5084	-0.1566	0.101*
C25	0.0723 (3)	0.41385 (16)	-0.06193 (15)	0.0704 (7)
H25	-0.0286	0.4058	-0.0557	0.084*
C26	0.1706 (2)	0.36411 (13)	-0.01120 (11)	0.0487 (5)
H26	0.1363	0.3224	0.0299	0.058*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0684 (9)	0.0398 (7)	0.0320 (6)	-0.0053 (6)	-0.0109 (6)	-0.0058 (5)
O2	0.0876 (10)	0.0251 (7)	0.0365 (7)	-0.0007 (6)	0.0008 (7)	-0.0003 (5)
N1	0.0420 (8)	0.0286 (7)	0.0280 (7)	-0.0001 (6)	-0.0064 (6)	0.0014 (6)
N2	0.0451 (8)	0.0256 (7)	0.0254 (7)	0.0015 (6)	0.0000 (6)	0.0024 (5)
C1	0.0534 (11)	0.0253 (8)	0.0255 (8)	-0.0046 (8)	-0.0026 (7)	0.0035 (7)
C2	0.0494 (11)	0.0275 (9)	0.0277 (8)	0.0007 (8)	-0.0044 (7)	0.0003 (7)
C3	0.0496 (10)	0.0258 (8)	0.0251 (8)	0.0005 (7)	-0.0003 (7)	-0.0025 (6)
C4	0.0616 (12)	0.0328 (9)	0.0283 (9)	0.0048 (9)	0.0038 (8)	-0.0028 (7)
C5	0.0664 (14)	0.0411 (11)	0.0381 (10)	0.0129 (10)	0.0013 (9)	-0.0056 (8)
C6	0.0641 (15)	0.0742 (16)	0.0593 (13)	-0.0053 (12)	0.0039 (11)	-0.0084 (12)
C7	0.0322 (9)	0.0282 (8)	0.0277 (8)	-0.0006 (7)	0.0018 (7)	-0.0014 (6)
C8	0.0338 (9)	0.0250 (8)	0.0268 (8)	0.0005 (7)	0.0042 (7)	-0.0010 (6)
C9	0.0353 (9)	0.0374 (10)	0.0267 (8)	0.0040 (7)	-0.0012 (7)	-0.0031 (7)
C10	0.0361 (10)	0.0390 (10)	0.0363 (9)	-0.0002 (8)	0.0008 (7)	-0.0131 (8)

supplementary materials

C11	0.0394 (10)	0.0270 (8)	0.0425 (10)	0.0000 (7)	0.0090 (8)	-0.0064 (7)
C12	0.0365 (9)	0.0287 (9)	0.0343 (9)	0.0029 (7)	0.0040 (7)	0.0029 (7)
C13	0.0466 (11)	0.0368 (10)	0.0379 (9)	0.0003 (8)	-0.0112 (8)	0.0053 (8)
C14	0.0378 (10)	0.0328 (9)	0.0430 (10)	-0.0051 (8)	-0.0135 (8)	0.0008 (8)
C15	0.0398 (11)	0.0435 (11)	0.0613 (12)	-0.0011 (9)	-0.0048 (9)	0.0144 (9)
C16	0.0472 (12)	0.0683 (15)	0.0654 (14)	-0.0086 (11)	0.0005 (10)	0.0253 (11)
C17	0.0401 (12)	0.0711 (15)	0.0707 (14)	-0.0050 (11)	0.0047 (10)	0.0036 (12)
C18	0.0400 (11)	0.0509 (13)	0.0779 (15)	0.0021 (9)	-0.0041 (11)	-0.0037 (11)
C19	0.0426 (11)	0.0368 (10)	0.0572 (12)	-0.0012 (9)	-0.0127 (9)	0.0023 (9)
C20	0.0502 (11)	0.0339 (9)	0.0302 (8)	-0.0051 (8)	0.0038 (8)	0.0057 (7)
C21	0.0631 (13)	0.0280 (9)	0.0243 (8)	0.0036 (8)	-0.0005 (8)	-0.0006 (7)
C22	0.0937 (16)	0.0383 (11)	0.0345 (10)	0.0081 (11)	0.0103 (10)	0.0069 (8)
C23	0.141 (3)	0.0484 (14)	0.0396 (12)	0.0187 (16)	0.0015 (14)	0.0142 (10)
C24	0.132 (3)	0.0580 (16)	0.0587 (15)	0.0313 (17)	-0.0366 (17)	0.0071 (12)
C25	0.0779 (16)	0.0554 (14)	0.0756 (16)	0.0177 (12)	-0.0285 (13)	-0.0023 (12)
C26	0.0633 (14)	0.0394 (11)	0.0425 (10)	0.0056 (10)	-0.0105 (9)	0.0016 (8)

Geometric parameters (Å, °)

O1—C1	1.2271 (19)	C13—C14	1.509 (2)
O2—C2	1.2216 (19)	C13—H13A	0.9900
N1—C1	1.367 (2)	C13—H13B	0.9900
N1—C7	1.4321 (19)	C14—C15	1.383 (2)
N1—C13	1.475 (2)	C14—C19	1.388 (2)
N2—C2	1.3678 (19)	C15—C16	1.388 (3)
N2—C8	1.4273 (19)	C15—H15	0.9500
N2—C20	1.4710 (19)	C16—C17	1.377 (3)
C1—C3	1.516 (2)	C16—H16	0.9500
C2—C3	1.529 (2)	C17—C18	1.371 (3)
C3—C4	1.521 (2)	C17—H17	0.9500
C3—H3	1.0000	C18—C19	1.385 (3)
C4—C5	1.496 (3)	C18—H18	0.9500
C4—H4A	0.9900	C19—H19	0.9500
C4—H4B	0.9900	C20—C21	1.506 (2)
C5—C6	1.300 (3)	C20—H20A	0.9900
C5—H5	0.9500	C20—H20B	0.9900
C6—H6A	0.9500	C21—C26	1.376 (3)
C6—H6B	0.9500	C21—C22	1.393 (2)
C7—C12	1.393 (2)	C22—C23	1.380 (3)
C7—C8	1.400 (2)	C22—H22	0.9500
C8—C9	1.392 (2)	C23—C24	1.372 (4)
C9—C10	1.376 (2)	C23—H23	0.9500
C9—H9	0.9500	C24—C25	1.381 (4)
C10—C11	1.385 (2)	C24—H24	0.9500
C10—H10	0.9500	C25—C26	1.392 (3)
C11—C12	1.376 (2)	C25—H25	0.9500
C11—H11	0.9500	C26—H26	0.9500
C12—H12	0.9500		
C1—N1—C7	122.36 (14)	N1—C13—C14	112.15 (13)

C1—N1—C13	119.35 (13)	N1—C13—H13A	109.2
C7—N1—C13	118.29 (13)	C14—C13—H13A	109.2
C2—N2—C8	122.66 (13)	N1—C13—H13B	109.2
C2—N2—C20	117.67 (13)	C14—C13—H13B	109.2
C8—N2—C20	119.58 (12)	H13A—C13—H13B	107.9
O1—C1—N1	123.00 (16)	C15—C14—C19	118.41 (17)
O1—C1—C3	121.99 (15)	C15—C14—C13	122.04 (16)
N1—C1—C3	114.85 (13)	C19—C14—C13	119.55 (16)
O2—C2—N2	121.55 (15)	C14—C15—C16	120.56 (18)
O2—C2—C3	122.56 (14)	C14—C15—H15	119.7
N2—C2—C3	115.74 (13)	C16—C15—H15	119.7
C1—C3—C4	112.72 (13)	C17—C16—C15	120.13 (19)
C1—C3—C2	102.56 (13)	C17—C16—H16	119.9
C4—C3—C2	112.70 (13)	C15—C16—H16	119.9
C1—C3—H3	109.5	C18—C17—C16	120.0 (2)
C4—C3—H3	109.5	C18—C17—H17	120.0
C2—C3—H3	109.5	C16—C17—H17	120.0
C5—C4—C3	112.65 (14)	C17—C18—C19	119.90 (19)
C5—C4—H4A	109.1	C17—C18—H18	120.1
C3—C4—H4A	109.1	C19—C18—H18	120.1
C5—C4—H4B	109.1	C18—C19—C14	120.98 (18)
C3—C4—H4B	109.1	C18—C19—H19	119.5
H4A—C4—H4B	107.8	C14—C19—H19	119.5
C6—C5—C4	126.20 (19)	N2—C20—C21	116.17 (14)
C6—C5—H5	116.9	N2—C20—H20A	108.2
C4—C5—H5	116.9	C21—C20—H20A	108.2
C5—C6—H6A	120.0	N2—C20—H20B	108.2
C5—C6—H6B	120.0	C21—C20—H20B	108.2
H6A—C6—H6B	120.0	H20A—C20—H20B	107.4
C12—C7—C8	119.37 (14)	C26—C21—C22	119.19 (18)
C12—C7—N1	119.39 (14)	C26—C21—C20	123.27 (15)
C8—C7—N1	121.20 (14)	C22—C21—C20	117.52 (18)
C9—C8—C7	119.02 (14)	C23—C22—C21	120.2 (2)
C9—C8—N2	119.64 (14)	C23—C22—H22	119.9
C7—C8—N2	121.34 (13)	C21—C22—H22	119.9
C10—C9—C8	120.93 (15)	C24—C23—C22	120.2 (2)
C10—C9—H9	119.5	C24—C23—H23	119.9
C8—C9—H9	119.5	C22—C23—H23	119.9
C9—C10—C11	119.97 (15)	C23—C24—C25	120.2 (2)
C9—C10—H10	120.0	C23—C24—H24	119.9
C11—C10—H10	120.0	C25—C24—H24	119.9
C12—C11—C10	119.91 (15)	C24—C25—C26	119.6 (3)
C12—C11—H11	120.0	C24—C25—H25	120.2
C10—C11—H11	120.0	C26—C25—H25	120.2
C11—C12—C7	120.77 (15)	C21—C26—C25	120.5 (2)
C11—C12—H12	119.6	C21—C26—H26	119.8
C7—C12—H12	119.6	C25—C26—H26	119.8
C7—N1—C1—O1	178.80 (15)	C7—C8—C9—C10	1.6 (2)
C13—N1—C1—O1	-0.6 (2)	N2—C8—C9—C10	-179.23 (15)

supplementary materials

C7—N1—C1—C3	-5.8 (2)	C8—C9—C10—C11	-0.3 (2)
C13—N1—C1—C3	174.81 (13)	C9—C10—C11—C12	-1.1 (2)
C8—N2—C2—O2	177.22 (16)	C10—C11—C12—C7	1.2 (2)
C20—N2—C2—O2	0.8 (2)	C8—C7—C12—C11	0.1 (2)
C8—N2—C2—C3	1.5 (2)	N1—C7—C12—C11	-177.57 (14)
C20—N2—C2—C3	-174.87 (14)	C1—N1—C13—C14	-124.15 (16)
O1—C1—C3—C4	-19.6 (2)	C7—N1—C13—C14	56.45 (19)
N1—C1—C3—C4	164.96 (14)	N1—C13—C14—C15	34.5 (2)
O1—C1—C3—C2	101.85 (17)	N1—C13—C14—C19	-146.39 (15)
N1—C1—C3—C2	-73.59 (16)	C19—C14—C15—C16	0.8 (3)
O2—C2—C3—C1	-99.46 (19)	C13—C14—C15—C16	179.95 (18)
N2—C2—C3—C1	76.21 (17)	C14—C15—C16—C17	-0.8 (3)
O2—C2—C3—C4	22.0 (2)	C15—C16—C17—C18	-0.3 (3)
N2—C2—C3—C4	-162.32 (14)	C16—C17—C18—C19	1.4 (3)
C1—C3—C4—C5	-171.39 (14)	C17—C18—C19—C14	-1.3 (3)
C2—C3—C4—C5	73.10 (19)	C15—C14—C19—C18	0.2 (3)
C3—C4—C5—C6	140.7 (2)	C13—C14—C19—C18	-178.88 (17)
C1—N1—C7—C12	-129.21 (16)	C2—N2—C20—C21	-71.74 (19)
C13—N1—C7—C12	50.2 (2)	C8—N2—C20—C21	111.77 (17)
C1—N1—C7—C8	53.2 (2)	N2—C20—C21—C26	-9.8 (2)
C13—N1—C7—C8	-127.46 (16)	N2—C20—C21—C22	171.75 (15)
C12—C7—C8—C9	-1.5 (2)	C26—C21—C22—C23	-1.0 (3)
N1—C7—C8—C9	176.16 (14)	C20—C21—C22—C23	177.51 (17)
C12—C7—C8—N2	179.35 (14)	C21—C22—C23—C24	-0.1 (3)
N1—C7—C8—N2	-3.0 (2)	C22—C23—C24—C25	1.0 (4)
C2—N2—C8—C9	134.46 (16)	C23—C24—C25—C26	-0.8 (4)
C20—N2—C8—C9	-49.2 (2)	C22—C21—C26—C25	1.2 (3)
C2—N2—C8—C7	-46.4 (2)	C20—C21—C26—C25	-177.19 (17)
C20—N2—C8—C7	129.94 (16)	C24—C25—C26—C21	-0.4 (3)

Fig. 1

