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5-Bromo-1-(prop-2-en-1-yl)-2,3-dihydro-1*H*-indole-2,3-dione

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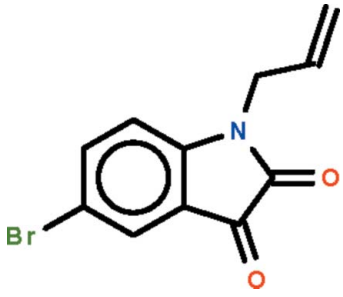
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.029; wR factor = 0.091; data-to-parameter ratio = 21.9.

In the title compound, $C_{11}H_8BrNO_2$, the nine-membered fused-ring is nearly planar [maximum deviation = 0.022 (2) Å] and the allyl group is arched over the nine-membered fused-ring at a dihedral angle of 89.2 (1)°. Weak intermolecular C—H···O hydrogen bonding is present in the crystal structure.

Related literature

For a related molecule, see: Abdel-Hamid *et al.* (2009).



Experimental

Crystal data

$C_{11}H_8BrNO_2$ M_r = 266.09
Orthorhombic, *Pccn*
a = 31.3411 (5) Å
b = 7.8995 (1) Å
c = 8.2716 (1) Å
V = 2047.87 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 3.99 mm^{-1}
T = 293 K
0.17 × 0.14 × 0.13 mm

Data collection

Bruker APEX DUO diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.550, T_{max} = 0.625
50850 measured reflections
2983 independent reflections
2345 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.091
S = 1.06
2983 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.41	3.273 (2)	154
C11—H11A···O2^{ii}	0.93	2.46	3.358 (3)	163

Symmetry codes: (i) $x, y-1, z$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

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).

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: XU5413).

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supporting information

Acta Cryst. (2012). E**68**, o240 [doi:10.1107/S160053681105447X]

5-Bromo-1-(prop-2-en-1-yl)-2,3-dihydro-1*H*-indole-2,3-dione

Khalil Maamri, Hafid Zouihri, El Mokhtar Essassi and Seik Weng Ng

S1. Comment

We are interested in the pharmaceutical properites of isatin derivatives; the allyl group 1-(prop-2-en-1-yl)-2,3-dihydro-1*H*-indole-2,3-dione, whose crystal structure was recently reported (Abdel-Hamid *et al.*, 2009), is a substituent that can undergo a variety of chemical transformation. The bromo-substituted title compound (Scheme I) features a planar fused-ring; the allyl group is arched over the five-membered ring (dihedral angle between allyl plane and nine-membered fused-ring 89.2 (1)°) (Fig. 1).

S2. Experimental

To a solution of 5-bromo-isatin (1g, 4.4 mmole) in *N*,*N*-dimethylformamide (50 ml) was added allyl bromide (1.50 g, 12.5 mmol) potassium carbonate (1 g, 7.4 mmol) along with a catalytic quantity of tetra-*n*-butylammonium bromide. The mixture was stirred for 48 h. The reaction was monitored by thin layer chromatography. The mixture was filtered and the solution evaporated under vacuum. The solid residue was recrystallized from ethanol to afford the title compound as red crystals.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C–H 0.93–0.97 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2*U*(C).

Omitted was the 2 0 0 reflection.

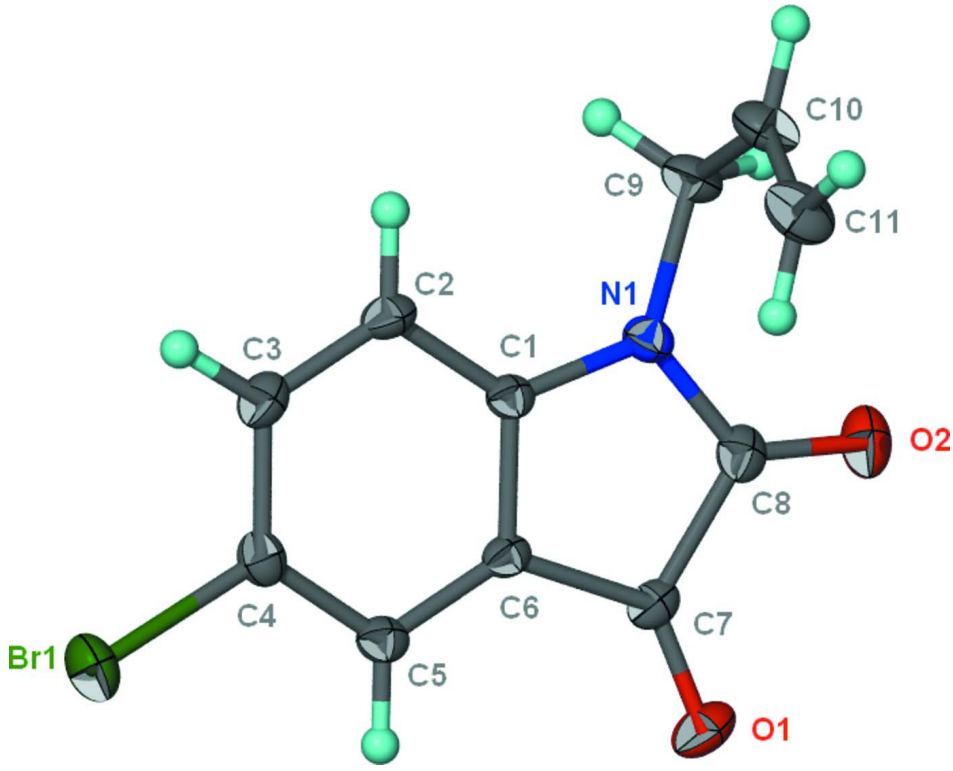

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $C_{11}H_8BrNO_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

5-Bromo-1-(prop-2-en-1-yl)-2,3-dihydro-1*H*-indole-2,3-dione

Crystal data

$C_{11}H_8BrNO_2$
$M_r = 266.09$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 31.3411\ (5)$ Å
$b = 7.8995\ (1)$ Å
$c = 8.2716\ (1)$ Å
$V = 2047.87\ (5)$ Å^3
$Z = 8$
$F(000) = 1056$
$D_x = 1.726$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9894 reflections
$\theta = 2.6–31.7°$
$\mu = 3.99$ mm^{-1}
$T = 293$ K
Prism, red
0.17 × 0.14 × 0.13 mm

Data collection

Bruker APEX DUO diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.550$, $T_{max} = 0.625$
50850 measured reflections
2983 independent reflections
2345 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.6°$
$h = -44\rightarrow44$
$k = -6\rightarrow11$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.091$
$S = 1.06$
2983 reflections
136 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
$w = 1/[\sigma^2(F_o^2) + (0.0456P)^2 + 1.4798P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.241206 (6)	0.49599 (3)	0.59089 (3)	0.03615 (9)
O1	0.12709 (5)	0.94850 (17)	0.22127 (18)	0.0334 (3)
O2	0.06568 (4)	0.77943 (19)	0.00288 (18)	0.0360 (3)
N1	0.09810 (5)	0.5408 (2)	0.10576 (18)	0.0237 (3)
C1	0.13156 (5)	0.5079 (2)	0.2140 (2)	0.0204 (3)
C2	0.14721 (6)	0.3526 (2)	0.2635 (2)	0.0253 (3)
H2	0.1358	0.2520	0.2242	0.030*
C3	0.18068 (6)	0.3522 (2)	0.3744 (2)	0.0270 (4)
H3	0.1919	0.2497	0.4098	0.032*
C4	0.19752 (6)	0.5033 (2)	0.4327 (2)	0.0250 (3)
C5	0.18246 (5)	0.6597 (2)	0.3816 (2)	0.0229 (3)
H5	0.1943	0.7602	0.4192	0.027*
C6	0.14914 (5)	0.6589 (2)	0.2724 (2)	0.0200 (3)
C7	0.12453 (5)	0.7978 (2)	0.2011 (2)	0.0229 (3)
C8	0.09146 (5)	0.7101 (2)	0.0887 (2)	0.0256 (4)
C9	0.07183 (6)	0.4118 (2)	0.0275 (2)	0.0295 (4)
H9A	0.0894	0.3138	0.0044	0.035*
H9B	0.0615	0.4560	−0.0748	0.035*
C10	0.03449 (6)	0.3572 (3)	0.1269 (3)	0.0342 (4)
H10	0.0177	0.2706	0.0850	0.041*
C11	0.02314 (7)	0.4189 (3)	0.2666 (3)	0.0379 (5)
H11A	0.0389	0.5057	0.3135	0.046*
H11B	−0.0008	0.3762	0.3193	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02822 (13)	0.04590 (15)	0.03435 (13)	0.00097 (8)	−0.00721 (7)	0.00370 (8)
O1	0.0391 (8)	0.0187 (6)	0.0424 (8)	0.0006 (6)	0.0109 (6)	0.0018 (6)
O2	0.0273 (6)	0.0407 (8)	0.0400 (8)	0.0049 (6)	−0.0013 (6)	0.0119 (6)
N1	0.0215 (7)	0.0233 (7)	0.0264 (7)	−0.0038 (6)	−0.0012 (6)	−0.0004 (6)
C1	0.0190 (7)	0.0200 (7)	0.0223 (7)	−0.0026 (6)	0.0031 (6)	−0.0009 (6)
C2	0.0287 (9)	0.0173 (7)	0.0300 (9)	−0.0020 (6)	0.0035 (7)	−0.0015 (6)
C3	0.0280 (8)	0.0237 (8)	0.0292 (8)	0.0033 (7)	0.0042 (7)	0.0033 (7)

C4	0.0205 (7)	0.0303 (9)	0.0240 (8)	−0.0001 (6)	0.0014 (6)	0.0017 (7)
C5	0.0215 (7)	0.0233 (8)	0.0238 (8)	−0.0034 (6)	0.0037 (6)	−0.0021 (6)
C6	0.0191 (7)	0.0167 (7)	0.0241 (8)	−0.0021 (6)	0.0054 (6)	−0.0009 (6)
C7	0.0233 (8)	0.0193 (7)	0.0261 (8)	−0.0006 (6)	0.0087 (6)	0.0013 (6)
C8	0.0203 (7)	0.0282 (8)	0.0283 (9)	−0.0002 (6)	0.0059 (6)	0.0041 (7)
C9	0.0274 (9)	0.0330 (9)	0.0280 (9)	−0.0077 (7)	−0.0016 (7)	−0.0066 (7)
C10	0.0303 (9)	0.0370 (10)	0.0353 (10)	−0.0142 (8)	−0.0030 (8)	−0.0007 (8)
C11	0.0307 (10)	0.0483 (13)	0.0348 (10)	−0.0133 (9)	0.0031 (8)	0.0024 (9)

Geometric parameters (Å, º)

Br1—C4	1.8950 (19)	C4—C5	1.388 (2)
O1—C7	1.205 (2)	C5—C6	1.381 (2)
O2—C8	1.207 (2)	C5—H5	0.9300
N1—C8	1.361 (2)	C6—C7	1.465 (2)
N1—C1	1.403 (2)	C7—C8	1.555 (3)
N1—C9	1.461 (2)	C9—C10	1.494 (3)
C1—C2	1.383 (2)	C9—H9A	0.9700
C1—C6	1.400 (2)	C9—H9B	0.9700
C2—C3	1.393 (3)	C10—C11	1.304 (3)
C2—H2	0.9300	C10—H10	0.9300
C3—C4	1.392 (3)	C11—H11A	0.9300
C3—H3	0.9300	C11—H11B	0.9300
C8—N1—C1	111.23 (14)	C1—C6—C7	107.00 (15)
C8—N1—C9	123.58 (16)	O1—C7—C6	130.50 (18)
C1—N1—C9	125.10 (15)	O1—C7—C8	124.55 (17)
C2—C1—C6	120.94 (16)	C6—C7—C8	104.94 (14)
C2—C1—N1	128.18 (15)	O2—C8—N1	127.52 (18)
C6—C1—N1	110.88 (14)	O2—C8—C7	126.57 (17)
C1—C2—C3	117.64 (16)	N1—C8—C7	105.90 (15)
C1—C2—H2	121.2	N1—C9—C10	113.51 (16)
C3—C2—H2	121.2	N1—C9—H9A	108.9
C2—C3—C4	120.78 (17)	C10—C9—H9A	108.9
C2—C3—H3	119.6	N1—C9—H9B	108.9
C4—C3—H3	119.6	C10—C9—H9B	108.9
C5—C4—C3	121.93 (17)	H9A—C9—H9B	107.7
C5—C4—Br1	118.89 (13)	C11—C10—C9	126.42 (19)
C3—C4—Br1	119.16 (13)	C11—C10—H10	116.8
C6—C5—C4	116.90 (16)	C9—C10—H10	116.8
C6—C5—H5	121.5	C10—C11—H11A	120.0
C4—C5—H5	121.5	C10—C11—H11B	120.0
C5—C6—C1	121.79 (15)	H11A—C11—H11B	120.0
C5—C6—C7	131.16 (15)		
C8—N1—C1—C2	179.10 (18)	N1—C1—C6—C7	1.88 (19)
C9—N1—C1—C2	2.4 (3)	C5—C6—C7—O1	−0.6 (3)
C8—N1—C1—C6	−0.8 (2)	C1—C6—C7—O1	176.84 (19)

C9—N1—C1—C6	−177.57 (16)	C5—C6—C7—C8	−179.54 (17)
C6—C1—C2—C3	0.6 (3)	C1—C6—C7—C8	−2.06 (17)
N1—C1—C2—C3	−179.32 (17)	C1—N1—C8—O2	178.62 (17)
C1—C2—C3—C4	0.1 (3)	C9—N1—C8—O2	−4.6 (3)
C2—C3—C4—C5	−1.1 (3)	C1—N1—C8—C7	−0.51 (19)
C2—C3—C4—Br1	177.05 (14)	C9—N1—C8—C7	176.28 (15)
C3—C4—C5—C6	1.4 (3)	O1—C7—C8—O2	3.5 (3)
Br1—C4—C5—C6	−176.78 (12)	C6—C7—C8—O2	−177.56 (17)
C4—C5—C6—C1	−0.7 (2)	O1—C7—C8—N1	−177.40 (17)
C4—C5—C6—C7	176.46 (17)	C6—C7—C8—N1	1.59 (18)
C2—C1—C6—C5	−0.3 (3)	C8—N1—C9—C10	−90.0 (2)
N1—C1—C6—C5	179.64 (15)	C1—N1—C9—C10	86.3 (2)
C2—C1—C6—C7	−178.08 (16)	N1—C9—C10—C11	3.6 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.93	2.41	3.273 (2)	154
C11—H11*A*···O2^{ii}	0.93	2.46	3.358 (3)	163

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, −*y*+3/2, *z*+1/2.