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

Khalil Maamri,<sup>a</sup> Hafid Zouihri,<sup>b</sup> El Mokhtar Essassi<sup>a</sup> and Seik Weng Ng<sup>c,d\*</sup>

<sup>a</sup>Laboratoire de Chimie Organique Hétérocyclique, Pôle de Compétences Pharmacochimie, Université Mohammed V-Agdal, BP 1014 Avenue Ibn Batout, Rabat, Morocco, <sup>b</sup>CNRST Division UATRS, Angle Allal Fassi/FAR, BP 8027 Hay Riad, Rabat, Morocco, <sup>c</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and <sup>d</sup>Chemistry Department, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia

Correspondence e-mail: seikweng@um.edu.my

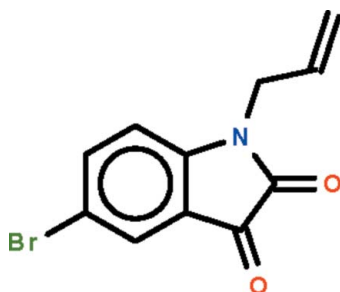
Received 17 December 2011; accepted 18 December 2011

Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.029;  $wR$  factor = 0.091; data-to-parameter ratio = 21.9.

In the title compound,  $\text{C}_{11}\text{H}_8\text{BrNO}_2$ , 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  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonding is present in the crystal structure.

Related literature

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



Experimental

Crystal data

$\text{C}_{11}\text{H}_8\text{BrNO}_2$

$M_r = 266.09$

Orthorhombic,  $Pccn$   
 $a = 31.3411$  (5) Å  
 $b = 7.8995$  (1) Å  
 $c = 8.2716$  (1) Å  
 $V = 2047.87$  (5) Å<sup>3</sup>

$Z = 8$   
 Mo  $K\alpha$  radiation  
 $\mu = 3.99$  mm<sup>-1</sup>  
 $T = 293$  K  
 $0.17 \times 0.14 \times 0.13$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$

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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.63$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C}2-\text{H}2\cdots\text{O}1^i$	0.93	2.41	3.273 (2)	154
$\text{C}11-\text{H}11A\cdots\text{O}2^{ii}$	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).

References

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**supplementary materials**

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

K. Maamri, H. Zouihri, E. M. Essassi and S. W. Ng

### Comment

We are interested in the pharmaceutical properties of isatin derivatives; the allyl group 1-(prop-2-en-1-yl)-2,3-dihydro-1H-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).

### 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.

### 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  $U(\text{H})$  set to  $1.2U(\text{C})$ .

Omitted was the 2 0 0 reflection.

### Figures

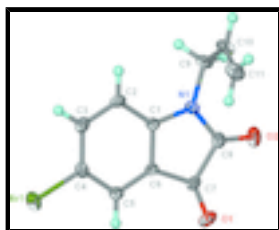


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of  $\text{C}_{11}\text{H}_8\text{BrNO}_2$  at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

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

### Crystal data

$\text{C}_{11}\text{H}_8\text{BrNO}_2$

$M_r = 266.09$

Orthorhombic, *Pccn*

$F(000) = 1056$

$D_x = 1.726 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

# supplementary materials

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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<sup>3</sup>  
 $Z = 8$

Cell parameters from 9894 reflections  
 $\theta = 2.6\text{--}31.7^\circ$   
 $\mu = 3.99$  mm<sup>-1</sup>  
 $T = 293$  K  
Prism, red  
 $0.17 \times 0.14 \times 0.13$  mm

## Data collection

Bruker APEX DUO  
diffractometer  
Radiation source: fine-focus sealed tube  
graphite  
 $\omega$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.035$   
 $\theta_{\max} = 30.0^\circ$ ,  $\theta_{\min} = 2.6^\circ$   
 $h = -44 \rightarrow 44$   
 $k = -6 \rightarrow 11$   
 $l = -11 \rightarrow 11$

## 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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.63$  e Å<sup>-3</sup>

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 ( $\text{\AA}$ ,  $^\circ$ )

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)

## supplementary materials

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 ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ O1 <sup>i</sup>	0.93	2.41	3.273 (2)	154
C11—H11A $\cdots$ O2 <sup>ii</sup>	0.93	2.46	3.358 (3)	163

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

Fig. 1

