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1-Propyl-1*H*-indole-2,3-dione

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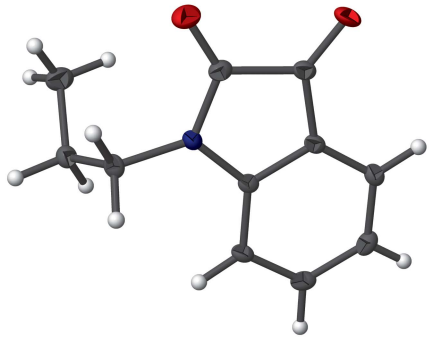
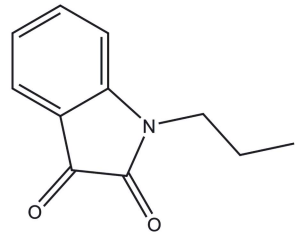
In the title compound, $C_{11}H_{11}NO_2$, the 1*H*-indole-2,3-dione unit is essentially planar, with an r.m.s. deviation of 0.0387 (13) Å. This plane makes a dihedral angle of 72.19 (17)° with the plane of the propyl substituent. In the crystal, chains propagating along the *b* axis are formed through C—H···O hydrogen bonds.

3D view



Chemical scheme



Structure description

Formerly, the study of isatin (1*H*-indole-2,3-dione) derivatives was connected with dye synthesis, but more recently these heterocycles have been shown to possess biological and pharmacological properties. They are also used as key intermediates in organic synthesis (da Silva *et al.*, 2001). Isatin is a core constituent of many alkaloids (Batanero & Barba, 2006) and drugs (Aboul-Fadl *et al.*, 2010) as well as dyes (Doménech *et al.*, 2009), pesticides and analytical reagents. Various derivatives of isatin show diverse biological activities including antibacterial (Kassab *et al.*, 2010), antifungal (Amal Raj *et al.*, 2003), antiviral (Jarrahpour *et al.*, 2007), anti-HIV (Bal *et al.*, 2005), anti-mycobacterial (Karalı *et al.*, 2007), anticancer (Gürsoy & Karalı 2003), and anti-inflammatory activities (Sridhar & Ramesh 2001) and are also effective anticonvulsants (Verma *et al.* 2004). Furthermore, isatin derivatives with their multifunctionality and diversity of transformations are synthetically versatile substrates and many efforts have been made toward the synthesis of these compounds.

In this work we report the synthesis and structure of a new derivative of isatin (Fig. 1) prepared by the action of 1-bromopropane alkyl on 1*H*-indole-2,3-dione in the presence of a catalytic quantity of tetra-*n*-butylammonium bromide. The near planarity of the

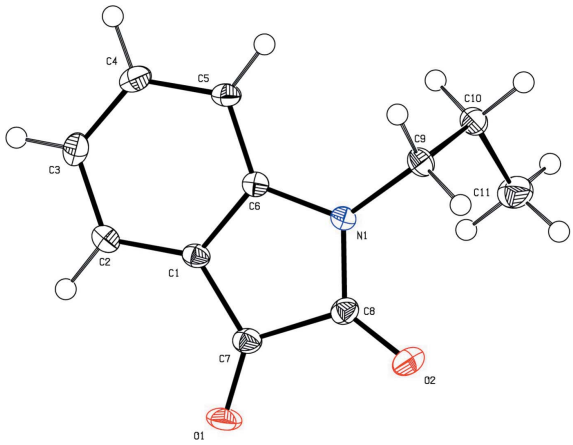


Figure 1
The molecular structure of the title molecule, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

isatin ring system is illustrated by a maximum deviation of 0.0387 (13) Å for the O2 atom from the best-fit plane through the 11 atoms of the ring system (Fig. 1). All bond lengths and angles compare well with those reported in the structure of 5-bromo-1-(prop-2-en-1-yl)-2, 3-dihydro-1*H*-indole-2, 3-dione (Maamri *et al.*, 2012).

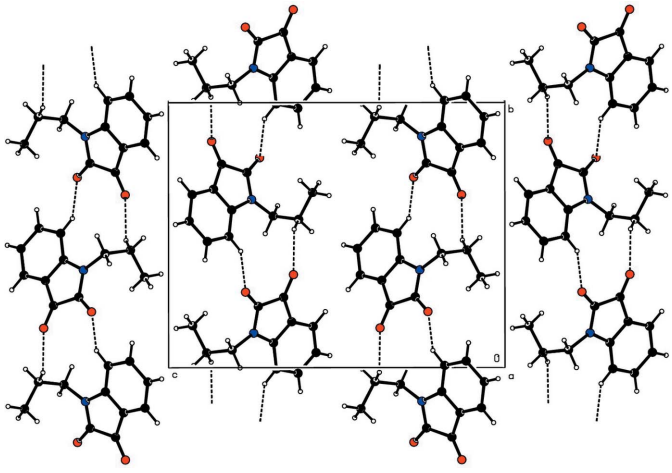


Figure 2
View along the *a* axis of the packing structure of the title compound. The dashed lines indicate intermolecular C—H···O interactions.

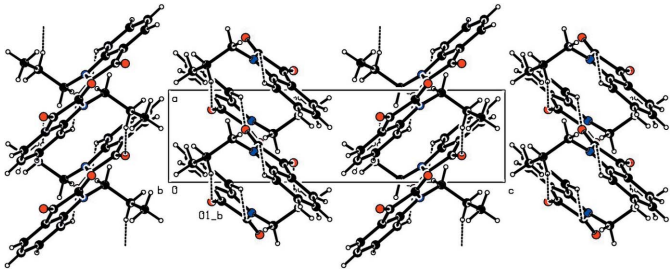


Figure 3
The crystal structure of the title compound, viewed along the *b* axis, showing chains parallel to the *b* axis of the unit cell.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.96 (2)	2.52 (2)	3.339 (2)	143.6 (16)
C10—H10*B*···O1^{ii}	0.96 (2)	2.57 (2)	3.439 (2)	149.4 (17)

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

Two C—H···O intermolecular hydrogen bonds are observed in the crystal structure, Table 1; they link molecules, forming parallel chains along the *b* axis (Figs. 2 and 3). π–π interactions are observed between the five- and six-membered rings of neighbouring molecules, with a $Cg1\cdots Cg2^{i}$ distance of 3.6218 (10) Å [Cg_1 and Cg_2 are the centroids of the (N1/C1/C6–C8) and (C1–C6) rings, respectively; symmetry code: (i): $1+x, y, z$].

Synthesis and crystallization

To a solution of isatin (0.2 g, 1.4 mmol) dissolved in DMF(10 ml) was added potassium carbonate (0.33 g, 2.38 mmol), a catalytic quantity of tetra-*n*-butylammonium bromide (0.04 g, 0.11 mmol) and 1-bromopropane (0.13 ml, 1.4 mmol). The mixture was stirred for 48 h; the reaction was monitored by thin layer chromatography. The mixture was filtered and the solvent removed under vacuum. The resulting

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{11}NO_2$
M_r	189.21
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, *b*, *c* (Å)	4.4666 (2), 12.9169 (6), 16.3857 (8)
V (Å^3)	945.37 (8)
Z	4
Radiation type	Mo *Kα*
μ (mm^{-1})	0.09
Crystal size (mm)	0.28 × 0.24 × 0.10
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.681, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8372, 2720, 2474
R_{int}	0.026
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.714
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.038, 0.089, 1.26
No. of reflections	2720
No. of parameters	171
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.21
Absolute structure	Flack *x* determined using 912 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.5 (5)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2010).

solid was recrystallized from ethanol to afford the title compound as red crystals in 82% yield (m.p. 357 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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full crystallographic data

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1-Propyl-1*H*-indole-2,3-dione

Crystal data

$C_{11}H_{11}NO_2$
M_r = 189.21
Orthorhombic, $P2_12_12_1$
a = 4.4666 (2) Å
b = 12.9169 (6) Å
c = 16.3857 (8) Å
V = 945.37 (8) Å^3
Z = 4
$F(000)$ = 400
D_x = 1.329 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3897 reflections
θ = 2.5–30.5°
μ = 0.09 mm^{-1}
T = 100 K
Parallelepiped, orange
0.28 × 0.24 × 0.10 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: microfocus source
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.681, T_{max} = 0.746
8372 measured reflections
2720 independent reflections
2474 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 30.5°, θ_{min} = 2.0°
h = −6→5
k = −17→12
l = −23→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.089
S = 1.25
2720 reflections
171 parameters
0 restraints
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack x determined using 912 quotients [(I+)-(I-)]/[(I+)+(I-)] (Parsons *et al.*, 2013)
Absolute structure parameter: −0.5 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C7	0.2074 (4)	0.23633 (14)	0.34207 (9)	0.0167 (3)
C5	0.0195 (4)	0.50779 (14)	0.32062 (10)	0.0161 (3)
C3	−0.2671 (4)	0.44800 (15)	0.43838 (10)	0.0200 (4)
C8	0.3971 (4)	0.26930 (14)	0.26673 (10)	0.0167 (3)
C1	0.0449 (3)	0.32977 (13)	0.36607 (9)	0.0145 (3)
C9	0.4709 (4)	0.43360 (15)	0.18883 (10)	0.0173 (3)
C10	0.2755 (4)	0.44538 (14)	0.11315 (10)	0.0179 (3)
C6	0.1282 (3)	0.40851 (13)	0.31200 (9)	0.0131 (3)
C4	−0.1806 (4)	0.52562 (14)	0.38456 (10)	0.0194 (4)
C2	−0.1525 (4)	0.34886 (14)	0.42971 (10)	0.0166 (3)
C11	0.2039 (5)	0.34352 (16)	0.07157 (12)	0.0270 (4)
N1	0.3325 (3)	0.37085 (11)	0.25297 (8)	0.0150 (3)
O1	0.2111 (3)	0.15078 (9)	0.37136 (7)	0.0235 (3)
O2	0.5712 (3)	0.21478 (10)	0.22898 (8)	0.0247 (3)
H2	−0.211 (5)	0.2930 (18)	0.4661 (14)	0.030 (6)*
H3	−0.405 (5)	0.4602 (16)	0.4792 (14)	0.029 (5)*
H4	−0.266 (5)	0.5948 (17)	0.3915 (12)	0.022 (5)*
H5	0.075 (4)	0.5642 (16)	0.2856 (13)	0.024 (5)*
H9A	0.666 (4)	0.3964 (15)	0.1758 (12)	0.016 (5)*
H9B	0.517 (4)	0.5007 (15)	0.2124 (11)	0.011 (4)*
H10B	0.093 (5)	0.4815 (16)	0.1264 (12)	0.023 (5)*
H10A	0.391 (4)	0.4923 (16)	0.0746 (12)	0.021 (5)*
H11A	0.084 (6)	0.3542 (16)	0.0226 (15)	0.034 (6)*
H11B	0.387 (6)	0.3080 (19)	0.0530 (15)	0.044 (7)*
H11C	0.084 (5)	0.2976 (17)	0.1088 (15)	0.031 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C7	0.0205 (8)	0.0129 (9)	0.0166 (7)	−0.0014 (6)	−0.0032 (6)	−0.0009 (6)
C5	0.0188 (7)	0.0114 (9)	0.0180 (7)	0.0000 (6)	−0.0027 (6)	0.0006 (6)
C3	0.0184 (8)	0.0257 (10)	0.0158 (7)	0.0029 (7)	0.0011 (6)	−0.0029 (7)
C8	0.0177 (7)	0.0160 (9)	0.0164 (7)	0.0015 (6)	−0.0020 (6)	−0.0023 (6)
C1	0.0160 (7)	0.0123 (9)	0.0151 (7)	−0.0012 (6)	−0.0030 (6)	0.0007 (6)
C9	0.0160 (7)	0.0181 (10)	0.0176 (7)	−0.0030 (7)	0.0020 (6)	0.0024 (6)
C10	0.0189 (7)	0.0180 (9)	0.0170 (7)	−0.0001 (7)	0.0004 (6)	0.0017 (7)
C6	0.0121 (6)	0.0130 (9)	0.0143 (6)	−0.0018 (6)	−0.0028 (6)	−0.0007 (6)
C4	0.0208 (8)	0.0159 (10)	0.0217 (8)	0.0042 (7)	−0.0034 (7)	−0.0033 (7)
C2	0.0172 (7)	0.0167 (9)	0.0159 (7)	−0.0023 (6)	−0.0016 (6)	0.0026 (6)
C11	0.0354 (10)	0.0226 (11)	0.0231 (9)	0.0029 (9)	−0.0061 (8)	−0.0039 (8)
N1	0.0179 (7)	0.0122 (8)	0.0148 (6)	−0.0001 (5)	0.0016 (5)	0.0012 (5)
O1	0.0353 (7)	0.0104 (7)	0.0247 (6)	0.0001 (5)	−0.0025 (5)	0.0032 (5)
O2	0.0291 (7)	0.0197 (8)	0.0253 (6)	0.0081 (6)	0.0024 (6)	−0.0027 (5)

Geometric parameters (Å, º)

C7—O1	1.205 (2)	C9—N1	1.464 (2)
C7—C1	1.462 (2)	C9—C10	1.524 (2)
C7—C8	1.557 (2)	C9—H9A	1.02 (2)
C5—C6	1.379 (2)	C9—H9B	0.971 (19)
C5—C4	1.396 (2)	C10—C11	1.516 (3)
C5—H5	0.96 (2)	C10—H10B	0.96 (2)
C3—C2	1.386 (3)	C10—H10A	1.02 (2)
C3—C4	1.390 (3)	C6—N1	1.416 (2)
C3—H3	0.92 (2)	C4—H4	0.98 (2)
C8—O2	1.218 (2)	C2—H2	0.97 (2)
C8—N1	1.362 (2)	C11—H11A	0.97 (2)
C1—C2	1.388 (2)	C11—H11B	0.98 (3)
C1—C6	1.399 (2)	C11—H11C	1.01 (2)
O1—C7—C1	131.04 (16)	C9—C10—H10B	110.4 (12)
O1—C7—C8	124.02 (16)	C11—C10—H10A	110.2 (12)
C1—C7—C8	104.93 (14)	C9—C10—H10A	106.0 (11)
C6—C5—C4	117.12 (16)	H10B—C10—H10A	106.2 (17)
C6—C5—H5	123.6 (12)	C5—C6—C1	121.17 (15)
C4—C5—H5	119.3 (12)	C5—C6—N1	128.07 (14)
C2—C3—C4	119.91 (16)	C1—C6—N1	110.75 (14)
C2—C3—H3	118.6 (13)	C3—C4—C5	122.35 (17)
C4—C3—H3	121.5 (13)	C3—C4—H4	118.5 (12)
O2—C8—N1	127.46 (16)	C5—C4—H4	119.2 (12)
O2—C8—C7	126.30 (16)	C1—C2—C3	118.41 (16)
N1—C8—C7	106.23 (13)	C1—C2—H2	119.9 (13)
C2—C1—C6	121.04 (16)	C3—C2—H2	121.7 (13)
C2—C1—C7	131.62 (16)	C10—C11—H11A	111.3 (12)
C6—C1—C7	107.31 (14)	C10—C11—H11B	111.7 (14)
N1—C9—C10	113.42 (13)	H11A—C11—H11B	105 (2)
N1—C9—H9A	104.5 (11)	C10—C11—H11C	110.6 (13)
C10—C9—H9A	111.5 (11)	H11A—C11—H11C	106.9 (19)
N1—C9—H9B	107.3 (11)	H11B—C11—H11C	110.7 (19)
C10—C9—H9B	110.8 (11)	C8—N1—C6	110.75 (13)
H9A—C9—H9B	108.9 (15)	C8—N1—C9	124.24 (14)
C11—C10—C9	113.57 (15)	C6—N1—C9	124.91 (14)
C11—C10—H10B	110.1 (12)		
O1—C7—C8—O2	−0.7 (3)	C2—C3—C4—C5	0.3 (3)
C1—C7—C8—O2	178.18 (16)	C6—C5—C4—C3	0.6 (2)
O1—C7—C8—N1	−179.65 (16)	C6—C1—C2—C3	0.3 (2)
C1—C7—C8—N1	−0.79 (17)	C7—C1—C2—C3	178.24 (17)
O1—C7—C1—C2	0.4 (3)	C4—C3—C2—C1	−0.8 (2)
C8—C7—C1—C2	−178.34 (16)	O2—C8—N1—C6	−177.48 (16)
O1—C7—C1—C6	178.56 (17)	C7—C8—N1—C6	1.48 (16)
C8—C7—C1—C6	−0.18 (17)	O2—C8—N1—C9	−1.0 (3)

N1—C9—C10—C11	−61.1 (2)	C7—C8—N1—C9	177.95 (13)
C4—C5—C6—C1	−1.1 (2)	C5—C6—N1—C8	177.01 (16)
C4—C5—C6—N1	−179.70 (15)	C1—C6—N1—C8	−1.69 (17)
C2—C1—C6—C5	0.7 (2)	C5—C6—N1—C9	0.6 (2)
C7—C1—C6—C5	−177.72 (14)	C1—C6—N1—C9	−178.13 (14)
C2—C1—C6—N1	179.48 (14)	C10—C9—N1—C8	99.75 (18)
C7—C1—C6—N1	1.09 (18)	C10—C9—N1—C6	−84.27 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···O2^{i}	0.96 (2)	2.52 (2)	3.339 (2)	143.6 (16)
C9—H9*A*···O2	1.018 (18)	2.538 (19)	2.936 (2)	102.8 (12)
C10—H10*B*···O1^{ii}	0.96 (2)	2.57 (2)	3.439 (2)	149.4 (17)

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