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3-(1,3-Dioxoisoindolin-2-yl)propanenitrile

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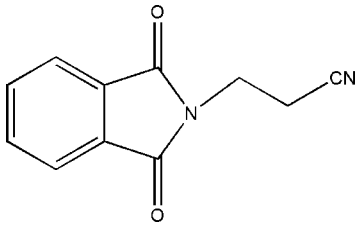
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.002 Å; R factor = 0.030; wR factor = 0.124; data-to-parameter ratio = 12.2.

In the title compound, $C_{11}H_8N_2O_2$, the packing is consolidated by C—H···N and C—H···O interactions.

Related literature

For related literature, see: Wingrove & Caret (1981).



Experimental

Crystal data

$C_{11}H_8N_2O_2$
M_r = 200.19
Monoclinic, $P2_1/c$
a = 9.1368 (17) Å
b = 8.2543 (16) Å
c = 12.646 (2) Å
β = 96.909 (3)°
V = 946.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 273 (2) K
0.17 × 0.15 × 0.12 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: none
4828 measured reflections
1674 independent reflections
1494 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.124
S = 1.00
1674 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11···N1^{i}	0.93	2.62	3.517 (2)	162
C8—H8···O2^{ii}	0.93	2.55	3.3922 (17)	151
C2—H2A···O1^{iii}	0.97	2.58	3.3682 (17)	138

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2669).

References

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Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
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supplementary materials

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3-(1,3-Dioxoisoindolin-2-yl)propanenitrile

X.-J. Li, M.-H. Xiong and C.-C. Xia

Comment

Isoindoline-1,3-dione derivatives exhibit a high level of biological activity (Wingrove & Caret, 1981). As a part of our studies in this area, we have isolated the title compound, (I), (Fig. 1).

As expected, the six-membered and five-membered rings are almost co-planar [dihedral angle = 0.67 (6)°]. In the crystal of (I), C—H···O and C—H···N interactions (Table 1) help to establish the packing (Fig. 2).

Experimental

Tht title compound was synthesized from a mixture of isoindoline-1,3-dione (5 mmol, 0.736 g) and 3-chloropropanenitrile (5 mmol, 0.448 g) and triethylamine (8 mmol, 0.505 g) and 30 ml *N*,*N*-dimethylformamide. The components were dissolved in 20 ml e thanol and 2 ml water, then heated to boiling and stirred for ten minutes. The system was cooled to the room temperature and colourless blocks of (I) were collected after six days.

Figures

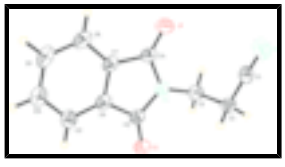

Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids for the non-hydrogen atoms.

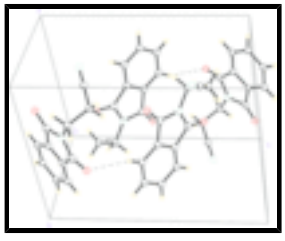

Fig. 2. Part of the crystal structure of (I), with hydrogen bonds shown as thin lines.

3-(1,3-Dioxoisoindolin-2-yl)propanenitrile

Crystal data

$C_{11}H_8N_2O_2$	F_{000} = 416
M_r = 200.19	D_x = 1.404 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2936 reflections
a = 9.1368 (17) Å	θ = 2.5–28.2º

b = 8.2543 (16) Å	μ = 0.10 mm^{-1}
c = 12.646 (2) Å	T = 273 (2) K
β = 96.909 (3)º	Block, colorless
V = 946.8 (3) Å^3	0.17 × 0.15 × 0.12 mm
Z = 4	

Data collection

Siemens SMART CCD diffractometer	1494 reflections with $I > 2\sigma(I)$
Radiation source: sealed tube	R_{int} = 0.018
Monochromator: graphite	θ_{max} = 25.0º
T = 273(2) K	θ_{min} = 3.0º
ω scans	h = −10→7
Absorption correction: none	k = −9→9
4828 measured reflections	l = −15→14
1674 independent reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.04P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.124	$(\Delta/\sigma)_{max}$ = 0.002
S = 1.00	$\Delta\rho_{max}$ = 0.13 e Å^{-3}
1674 reflections	$\Delta\rho_{min}$ = −0.12 e Å^{-3}
137 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.104 (13)
Secondary atom site location: difference Fourier map	

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.31079 (12)	0.24260 (12)	0.97960 (8)	0.0663 (4)
O2	0.56771 (10)	−0.04615 (12)	0.75807 (8)	0.0611 (3)
N1	0.05883 (14)	0.35783 (16)	0.75444 (12)	0.0732 (4)
N2	0.40733 (11)	0.08414 (11)	0.85568 (8)	0.0448 (3)
C1	0.12620 (14)	0.24940 (15)	0.73348 (11)	0.0510 (4)
C2	0.20664 (13)	0.10716 (16)	0.70665 (10)	0.0499 (4)
H2A	0.2848	0.1402	0.6658	0.060*
H2B	0.1405	0.0368	0.6619	0.060*
C3	0.27357 (14)	0.01227 (15)	0.80366 (10)	0.0496 (4)
H3A	0.2020	0.0053	0.8542	0.060*
H3B	0.2947	−0.0971	0.7819	0.060*
C4	0.41465 (14)	0.19575 (15)	0.93856 (9)	0.0469 (4)
C5	0.54539 (14)	0.04830 (14)	0.82728 (9)	0.0450 (3)
C6	0.65174 (14)	0.14708 (13)	0.89805 (9)	0.0456 (3)
C7	0.57276 (14)	0.23633 (14)	0.96403 (9)	0.0464 (4)
C8	0.64206 (17)	0.34173 (15)	1.03802 (10)	0.0586 (4)
H8	0.5890	0.4026	1.0822	0.070*
C9	0.79450 (19)	0.35366 (16)	1.04404 (11)	0.0659 (4)
H9	0.8443	0.4242	1.0932	0.079*
C10	0.87332 (18)	0.26370 (17)	0.97915 (12)	0.0649 (4)
H10	0.9754	0.2735	0.9855	0.078*
C11	0.80229 (15)	0.15797 (16)	0.90385 (11)	0.0573 (4)
H11	0.8549	0.0972	0.8593	0.069*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0719 (7)	0.0692 (7)	0.0603 (7)	0.0093 (5)	0.0179 (5)	−0.0101 (5)
O2	0.0645 (6)	0.0646 (6)	0.0544 (6)	0.0029 (4)	0.0073 (5)	−0.0196 (5)
N1	0.0610 (8)	0.0670 (8)	0.0897 (10)	0.0111 (6)	0.0017 (7)	−0.0017 (7)
N2	0.0512 (6)	0.0400 (5)	0.0433 (6)	−0.0014 (4)	0.0058 (4)	−0.0009 (4)
C1	0.0417 (7)	0.0532 (8)	0.0566 (8)	−0.0056 (5)	0.0001 (6)	0.0029 (5)
C2	0.0500 (7)	0.0527 (7)	0.0472 (7)	−0.0050 (5)	0.0060 (5)	−0.0037 (5)
C3	0.0528 (7)	0.0415 (6)	0.0547 (7)	−0.0060 (5)	0.0067 (6)	0.0008 (5)
C4	0.0619 (8)	0.0396 (6)	0.0401 (6)	0.0054 (5)	0.0097 (5)	0.0029 (5)
C5	0.0543 (7)	0.0414 (6)	0.0392 (6)	0.0015 (5)	0.0049 (5)	0.0013 (5)
C6	0.0576 (7)	0.0392 (6)	0.0391 (6)	−0.0003 (5)	0.0017 (5)	0.0047 (5)
C7	0.0635 (8)	0.0375 (6)	0.0366 (6)	0.0025 (5)	−0.0004 (5)	0.0046 (4)
C8	0.0843 (10)	0.0435 (7)	0.0449 (7)	0.0032 (6)	−0.0047 (6)	−0.0015 (5)
C9	0.0839 (10)	0.0508 (8)	0.0565 (8)	−0.0097 (7)	−0.0190 (7)	0.0016 (6)
C10	0.0660 (9)	0.0639 (9)	0.0610 (9)	−0.0114 (6)	−0.0083 (7)	0.0074 (7)
C11	0.0577 (8)	0.0581 (8)	0.0551 (8)	−0.0033 (6)	0.0030 (6)	0.0029 (6)

Geometric parameters (Å, °)

O1—C4	1.1992 (15)	C4—C7	1.4801 (18)
O2—C5	1.2076 (14)	C5—C6	1.4835 (17)
N1—C1	1.1356 (17)	C6—C11	1.3717 (18)
N2—C5	1.3845 (16)	C6—C7	1.3801 (17)
N2—C4	1.3910 (16)	C7—C8	1.3751 (17)
N2—C3	1.4440 (15)	C8—C9	1.389 (2)
C1—C2	1.4469 (18)	C8—H8	0.9300
C2—C3	1.5206 (18)	C9—C10	1.373 (2)
C2—H2A	0.9700	C9—H9	0.9300
C2—H2B	0.9700	C10—C11	1.3932 (19)
C3—H3A	0.9700	C10—H10	0.9300
C3—H3B	0.9700	C11—H11	0.9300
C5—N2—C4	111.98 (10)	O2—C5—C6	129.54 (11)
C5—N2—C3	122.80 (10)	N2—C5—C6	106.09 (10)
C4—N2—C3	125.22 (10)	C11—C6—C7	121.78 (12)
N1—C1—C2	177.64 (14)	C11—C6—C5	130.40 (11)
C1—C2—C3	113.27 (11)	C7—C6—C5	107.82 (11)
C1—C2—H2A	108.9	C8—C7—C6	121.18 (13)
C3—C2—H2A	108.9	C8—C7—C4	130.45 (12)
C1—C2—H2B	108.9	C6—C7—C4	108.37 (11)
C3—C2—H2B	108.9	C7—C8—C9	117.30 (13)
H2A—C2—H2B	107.7	C7—C8—H8	121.3
N2—C3—C2	113.09 (9)	C9—C8—H8	121.3
N2—C3—H3A	109.0	C10—C9—C8	121.56 (13)
C2—C3—H3A	109.0	C10—C9—H9	119.2
N2—C3—H3B	109.0	C8—C9—H9	119.2
C2—C3—H3B	109.0	C9—C10—C11	120.83 (15)
H3A—C3—H3B	107.8	C9—C10—H10	119.6
O1—C4—N2	124.81 (12)	C11—C10—H10	119.6
O1—C4—C7	129.44 (12)	C6—C11—C10	117.34 (13)
N2—C4—C7	105.73 (10)	C6—C11—H11	121.3
O2—C5—N2	124.37 (11)	C10—C11—H11	121.3
C5—N2—C3—C2	−88.43 (14)	C11—C6—C7—C8	0.69 (17)
C4—N2—C3—C2	91.44 (14)	C5—C6—C7—C8	−179.16 (10)
C1—C2—C3—N2	−78.45 (14)	C11—C6—C7—C4	−179.38 (10)
C5—N2—C4—O1	−177.63 (11)	C5—C6—C7—C4	0.77 (12)
C3—N2—C4—O1	2.48 (19)	O1—C4—C7—C8	−2.7 (2)
C5—N2—C4—C7	0.90 (13)	N2—C4—C7—C8	178.90 (11)
C3—N2—C4—C7	−178.99 (10)	O1—C4—C7—C6	177.41 (12)
C4—N2—C5—O2	179.38 (11)	N2—C4—C7—C6	−1.02 (13)
C3—N2—C5—O2	−0.73 (18)	C6—C7—C8—C9	−0.46 (17)
C4—N2—C5—C6	−0.44 (13)	C4—C7—C8—C9	179.63 (12)
C3—N2—C5—C6	179.44 (10)	C7—C8—C9—C10	−0.21 (19)
O2—C5—C6—C11	0.1 (2)	C8—C9—C10—C11	0.7 (2)
N2—C5—C6—C11	179.93 (12)	C7—C6—C11—C10	−0.23 (18)
O2—C5—C6—C7	179.96 (12)	C5—C6—C11—C10	179.59 (12)

N2—C5—C6—C7	−0.23 (12)	C9—C10—C11—C6	−0.43 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···N1^{i}	0.93	2.62	3.517 (2)	162
C8—H8···O2^{ii}	0.93	2.55	3.3922 (17)	151
C2—H2A···O1^{iii}	0.97	2.58	3.3682 (17)	138

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

Fig. 1

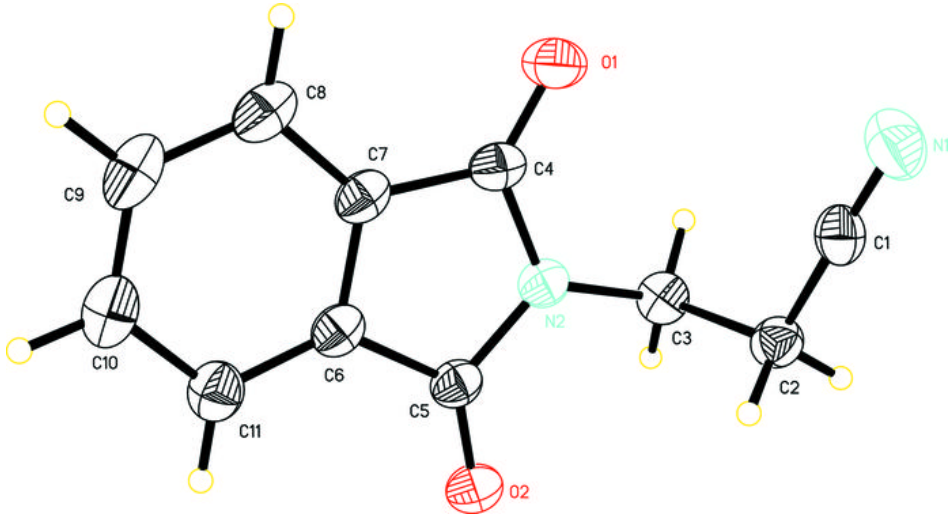

Fig. 2