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5-Amino-2-methylisoindoline-1,3-dione

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.134
Data-to-parameter ratio = 14.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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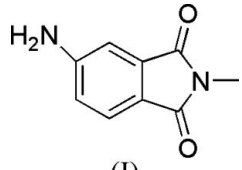
In the title molecule, $C_9H_8N_2O_2$, all non-H atoms are essentially coplanar. The crystal structure is stabilized by weak N—H···O hydrogen bonds.

Comment

The molecular structure of the title molecule, (I), is illustrated in Fig. 1. The molecule is planar to within 0.018 (2) Å for all non-H atoms. Geometric parameters are listed in Table 1. Considering the different substitution patterns, the geometry of the phthalimide ring system compares favourably with that in the related compounds *N*-aminophthalimide (Loehlin, 1985), and two isomeric nitrophthalimides (Glidewell *et al.*, 2004). The crystal structure is stabilized by weak N—H···O hydrogen bonds (Fig. 2 and Table 2).



(I)

Experimental

A mixture of $SnCl_2{\cdot}2H_2O$ (0.04 mol), hydrochloric acid (36%) (18 ml) and distilled water (15 ml) was stirred at room temperature for 15 min. 2-Methyl-5-nitroisoindoline-1,3-dione (0.01 mol) was then added and the mixture was stirred at 313 K for 3 h. After cooling and filtration, the title compound was recrystallized from ethanol (m.p. 520–522 K). 10 mg of (I) was dissolved in 15 ml dichloromethane, The solution was allowed to evaporate at room temperature and colourless single crystals were formed after 5 d.

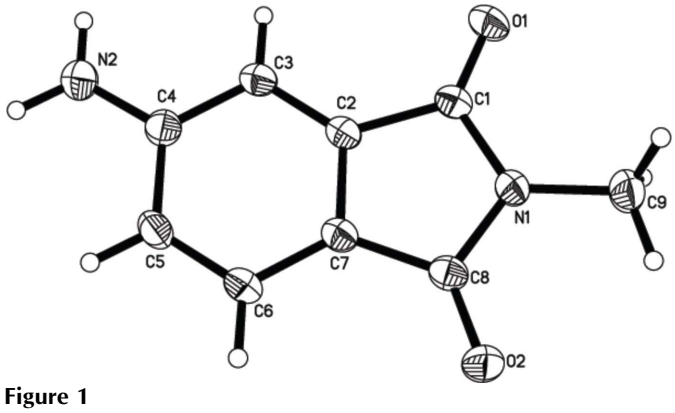


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

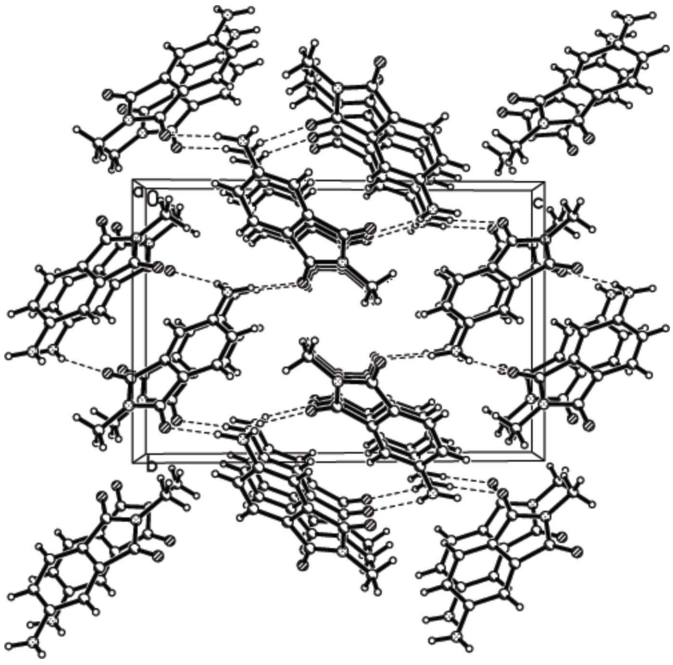


Figure 2
The packing of (I), viewed along the *a* axis. Dashed lines indicate hydrogen bonds.

Crystal data

$C_9H_8N_2O_2$
M_r = 176.17
Monoclinic, $P2_1/n$
a = 4.8300 (8) Å
b = 10.6480 (14) Å
c = 15.6476 (16) Å
β = 94.434 (9)°
V = 802.35 (19) Å^3
Z = 4
D_x = 1.458 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
Plate, colourless
0.22 × 0.20 × 0.06 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.972, T_{max} = 0.994
5949 measured reflections
1897 independent reflections
1447 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 27.8°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.134
S = 1.07
1897 reflections
128 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0796P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.144 (18)

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.2128 (19)	C2—C3	1.372 (2)
O2—C8	1.2228 (19)	C2—C7	1.395 (2)
N1—C1	1.393 (2)	C3—C4	1.410 (2)
N1—C8	1.396 (2)	C4—C5	1.409 (2)
N1—C9	1.452 (2)	C5—C6	1.375 (2)
N2—C4	1.370 (2)	C6—C7	1.387 (2)
C1—C2	1.495 (2)	C7—C8	1.465 (2)
C1—N1—C8	111.68 (13)	N2—C4—C3	120.39 (16)
C1—N1—C9	123.84 (14)	C5—C4—C3	119.47 (15)
C8—N1—C9	124.48 (13)	C6—C5—C4	121.76 (15)
O1—C1—N1	124.65 (15)	C5—C6—C7	118.48 (15)
O1—C1—C2	129.50 (15)	C6—C7—C2	120.10 (14)
N1—C1—C2	105.86 (13)	C6—C7—C8	131.35 (14)
C3—C2—C7	122.45 (14)	C2—C7—C8	108.55 (13)
C3—C2—C1	130.16 (14)	O2—C8—N1	123.80 (14)
C7—C2—C1	107.38 (13)	O2—C8—C7	129.71 (14)
C2—C3—C4	117.73 (15)	N1—C8—C7	106.49 (12)
N2—C4—C5	120.14 (16)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O2^{i}	0.93 (2)	2.39 (2)	3.252 (2)	154.2 (17)
N2—H2···O1^{ii}	0.84 (3)	2.39 (3)	3.179 (2)	156 (2)

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

H atoms bonded to C atoms were positioned geometrically, with C—H = 0.93–0.96 Å, and refined in the riding-model approximation, with U_{iso}(H) = 1.2U_{eq}(C). H atoms bonded to N atoms were refined independently with isotropic displacement parameters.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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