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## Key indicators

Single-crystal X-ray study  
 $T = 296$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.032  
 $wR$  factor = 0.079  
Data-to-parameter ratio = 6.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

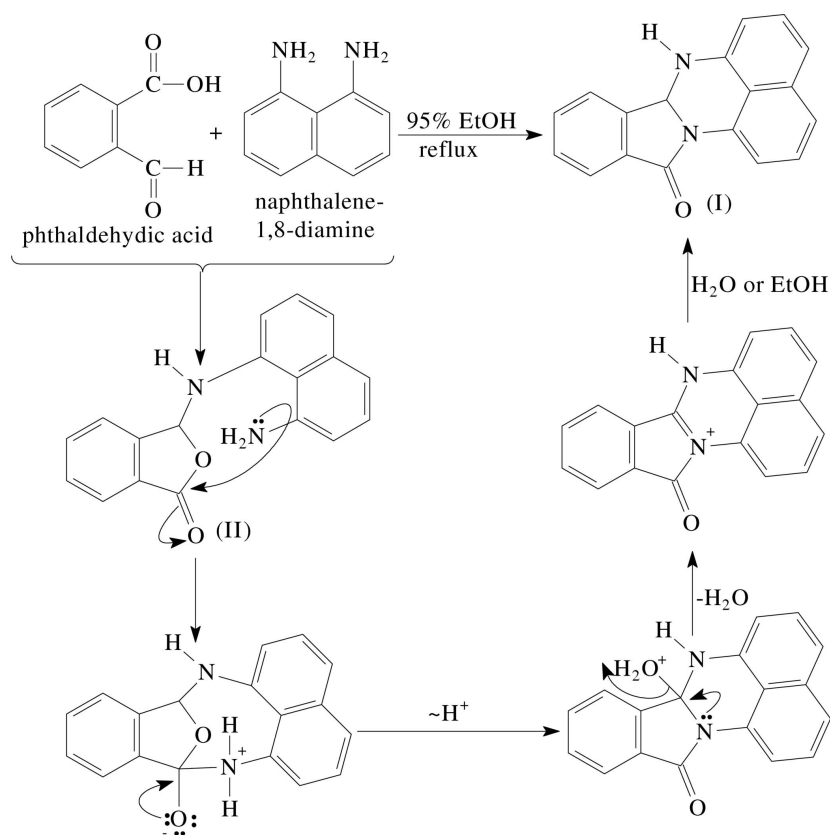
## 7,7a-Dihydroisoindolo[2,1-a]pyrimidin-12-one

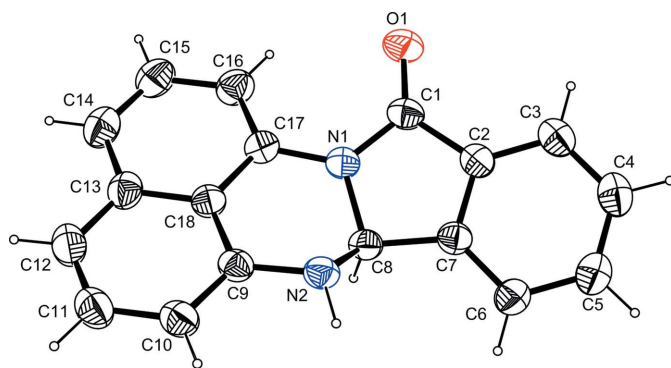
The crystal structure of the title compound,  $\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}$ , is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds and  $\text{C}-\text{H}\cdots\pi$  interactions.  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds generate a  $C(6)$  chain. The dihedral angle between the isoindoline group and the naphthalene ring system is  $24.96$  ( $12$ )°.

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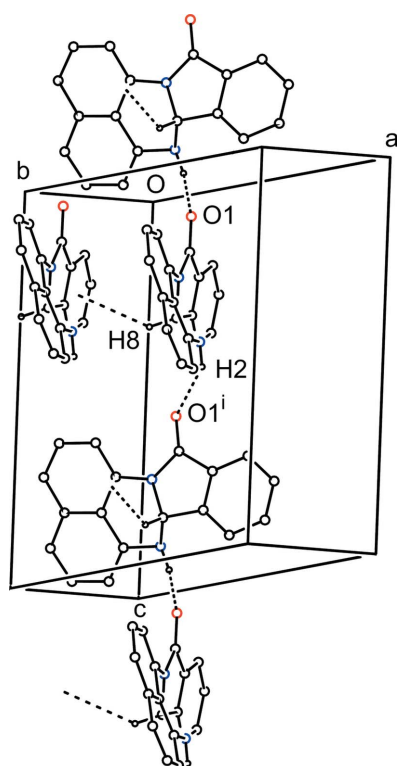
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## Comment

The present work is part of a structural study of compounds of 3-substituted phthalides (Odabaşoğlu & Büyükgüngör, 2006). When we used phthalaldehydic acid (2-formylbenzoic acid) and naphthalene-1,8-diamine as starting materials, aiming to synthesize 3-[(8-aminonaphthalen-1-yl)methyl]isobenzofuran-1(3*H*)-one, (II), we obtained the title compound, (I), unexpectedly (Fig. 1 and Table 1).The isoindoline group (C1–C8/N1) and naphthalene ring system are planar, the largest deviations from the mean planes being 0.029 (2) and 0.012 (3) Å for atoms N1 and C10, respectively. The crystal packing is stabilized by intermolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, which generate a  $C(6)$  chain (Etter, 1990), and also by  $\text{C}-\text{H}\cdots\text{Cg}1$  interactions ( $\text{Cg}1$



**Figure 1**  
A view of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 50% probability level.



**Figure 2**  
A packing diagram for (I), showing the N–H...O and C–H... $\pi$  interactions as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry code: (i)  $\frac{1}{2} - x, y, \frac{1}{2} + z$ .]

is the C2–C7 ring centroid; Fig. 2 and Table 2). The dihedral angle between the isoindoline group and the naphthalene ring system is 24.96 (12)°.

## Experimental

The title compound was prepared (see scheme in *Comment*) as described by Odabaşoğlu & Büyükgüngör (2006) using phthalaldehydic acid (2-formylbenzoic acid) and naphthalene-1,8-diamine as starting materials (yield 95%; m.p. 534–535 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.

## Crystal data

$C_{18}H_{12}N_2O$   
 $M_r = 272.30$   
Orthorhombic,  $Pca2_1$   
 $a = 19.8550$  (13) Å  
 $b = 4.7939$  (3) Å  
 $c = 13.6612$  (13) Å  
 $V = 1300.31$  (17) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.391$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 296$  K  
Plate, light brown  
 $0.62 \times 0.47 \times 0.21$  mm

## Data collection

Stoe IPDS-2 diffractometer  
 $\omega$  scans  
Absorption correction: integration  
(*X-RED32*; Stoe & Cie, 2002)  
 $T_{\min} = 0.945$ ,  $T_{\max} = 0.981$

12797 measured reflections  
1327 independent reflections  
1146 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.050$   
 $\theta_{\max} = 26.0^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.032$   
 $wR(F^2) = 0.079$   
 $S = 1.01$   
1327 reflections  
195 parameters  
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.056P)^2]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.11$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.14$  e Å<sup>-3</sup>  
Extinction correction: *SHELXL97*  
Extinction coefficient: 0.022 (3)

**Table 1**

Selected geometric parameters (Å, °).

C1–O1	1.228 (3)	C8–N1	1.466 (3)
C1–N1	1.362 (3)	C9–N2	1.408 (3)
C8–N2	1.443 (3)	C17–N1	1.405 (3)
N1–C1–C2	106.14 (19)	N1–C8–C7	102.40 (17)
N2–C8–N1	108.83 (15)	C1–N1–C17	129.75 (19)
N2–C8–C7	114.97 (19)	C9–N2–C8	112.93 (18)
C16–C17–N1–C1	23.2 (4)	C7–C8–N2–C9	170.29 (17)
N2–C8–N1–C17	–52.9 (2)		

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2–H2...O1 <sup>i</sup>	0.89 (3)	2.17 (3)	2.959 (3)	148 (2)
C8–H8...Cg1 <sup>ii</sup>	0.98	2.80	3.568	136

Symmetry codes: (i)  $-x + \frac{1}{2}, y, z + \frac{1}{2}$ ; (ii)  $x + \frac{1}{2}, -y + 1, z$ . Cg1 is the C2–C7 ring centroid.

In the absence of significant anomalous scattering effects, Friedel pairs were averaged. All H atoms attached to C atoms were treated as riding on their parent atoms, with C–H = 0.93 Å for aromatic H atoms and 0.98 Å for methine H atoms, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atom of the amino group was located in a difference Fourier map and freely refined.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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