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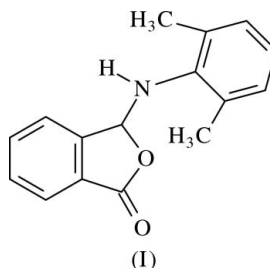
Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(C-C) = 0.006$ Å
 R factor = 0.057
 wR factor = 0.121
Data-to-parameter ratio = 14.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.3-(2,6-Dimethylanilino)isobenzofuran-1(3*H*)-one

The crystal structure of the title compound, $C_{16}H_{15}NO_2$, is stabilized by two $C-H \cdots O$ intermolecular hydrogen bonds. $C-H \cdots O$ hydrogen bonds which generate $C(6)$ chains and $R_3^3(14)$ motifs. The phthalide ring system of the molecule is almost planar and forms a dihedral angle of $51.7(2)^\circ$ with the benzene ring.

Comment

The present work is part of a structural study of compounds of 3-substituted phthalides and we report here the structure of 3-(2,6-dimethylanilino)isobenzofuran-1(3*H*)-one, (I) (Fig. 1).



The phthalide group ($C1-C8/O2$) is essentially planar, the largest deviation from the mean plane being $0.009(2)$ Å for atom $O2$. The dihedral angle between the mean planes of the phthalide group and the 2,6-dimethylphenyl ring is $51.7(2)^\circ$.

The crystal packing is stabilized by $C-H \cdots O$ intermolecular hydrogen bonds, which generate a $C(6)$ chain and $R_3^3(14)$ motifs (Etter, 1990). The title compound does not have an $N-H \cdots O$ hydrogen bond (Table 1), as also observed previously in 3-(4-methylpiperidin-1-yl)phthalide (Büyükgüngör & Odabaşoğlu, 2006) and 3-(2-hydroxy-5-methyl-anilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006a).

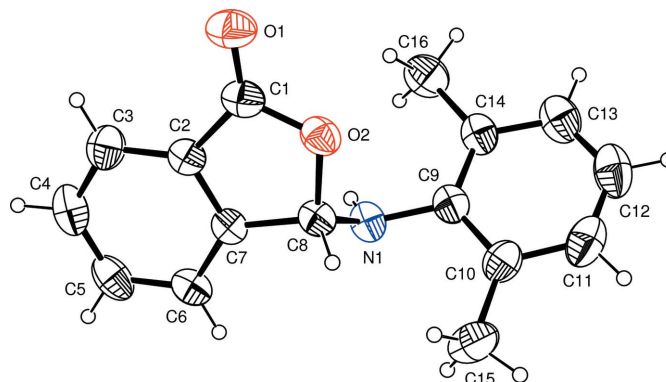


Figure 1

A view of (I) showing the atomic numbering scheme with displacement ellipsoids drawn at the 30% probability level.

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Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006*b*), using phthalaldehydic acid and 4-bromoaniline as starting materials (yield 81%, mp. 334–336 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

Crystal data

$C_{16}H_{15}NO_2$	$Z = 4$
$M_r = 253.29$	$D_x = 1.261 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 4.5301 (7) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$b = 23.424 (2) \text{ \AA}$	$T = 296 \text{ K}$
$c = 12.5843 (19) \text{ \AA}$	Plate, colorless
$\beta = 92.520 (12)^\circ$	$0.77 \times 0.29 \times 0.02 \text{ mm}$
$V = 1334.1 (3) \text{ \AA}^3$	

Data collection

Stoe IPDS-II diffractometer	2492 independent reflections
ω scans	923 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.144$
15246 measured reflections	$\theta_{\text{max}} = 25.5^\circ$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.057$	$w = 1/[\sigma^2(F_o^2) + (0.036P)^2]$
$wR(F^2) = 0.121$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.88$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2492 reflections	$\Delta\rho_{\text{max}} = 0.12 \text{ e \AA}^{-3}$
176 parameters	$\Delta\rho_{\text{min}} = -0.12 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C6-H6 \cdots O1^i$	0.93	2.58	3.255 (5)	130
$C6-H6 \cdots O1^{ii}$	0.93	2.89	3.294 (5)	108

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

The crystal of the light-atom compound was very thin (0.02 mm) and no better crystal was available. Therefore, although the selected exposure time was rather long (5 min), the diffraction was very weak, resulting in the low number of observed reflections and high value of $R_{\text{int}} = 0.144$. All H atoms attached to C atoms were treated as riding

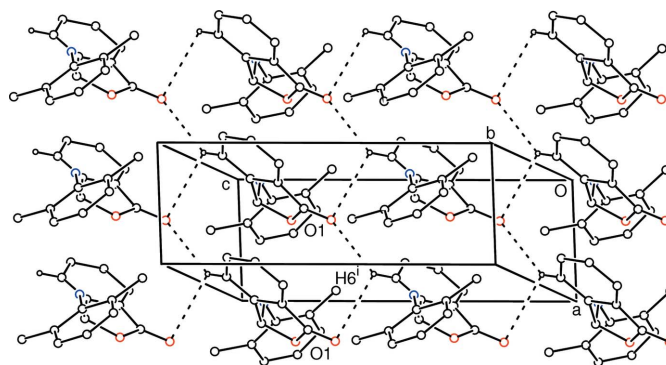


Figure 2

Part of the crystal structure of (I), showing the formation of hydrogen-bonded (dashed lines) $C(6)$ chains and $R_3^2(14)$ rings. H atoms not involved in hydrogen bonds have been omitted for clarity [Symmetry code: (i) $x + 1, y, z - \frac{1}{2}$].

on their parent atoms, with $C-H = 0.93-0.98 \text{ \AA}$, and with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$. The H atom of the amino group was located in a Fourier difference 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, 1990); 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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