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3-(4-Acetylanilino)isobenzofuran-1(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.071
Data-to-parameter ratio = 7.0

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

The crystal structure of the title compound, $C_{16}H_{13}NO_3$, is stabilized by an N—H···O and three C—H···O intermolecular hydrogen bonds and by C—H··· π interactions. The intermolecular hydrogen bonds generate $R_4^4(33)$ and $R_4^4(29)$ ring motifs. These hydrogen-bonded rings are linked *via* *C*(3) chains, generating a three-dimensional framework.

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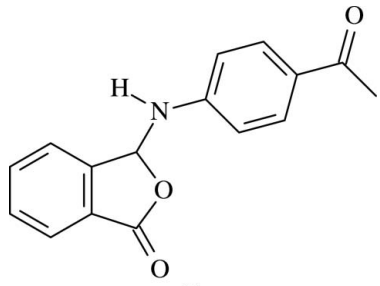
3-Substituted phthalides, Part XVII

Comment

Benzolactones are found in plants and they show several pharmacological effects, such as fungicidal, bactericidal, herbicidal and analgesic activities (Aoki *et al.*, 1973; Lacova, 1973). We report here the structure of 3-(4-acetylanilino)isobenzofuran-1(3*H*)-one, (I) (Fig. 1 and Table 1), as part of our systematic analysis of the structures of 3-substituted phthalides (3-substituted benzolactones).



(I)

In (I), the phthalide group (C1–C8/O2) is essentially planar, the largest deviation from the mean plane being 0.033 (2) Å for atom O2. The dihedral angle between the mean planes of the phthalide group and the benzene ring is 54.55 (10)°, which compares with 75.58 (15)° in 3-(4-chloroanilino)phthalide (Büyükgüngör & Odabaşoğlu, 2006), 74.10 (9)° in 3-(4-fluoroanilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*a*), 62.2 (2)° in 3-(4-bromoanilino)phthalide (Odabaşoğlu &

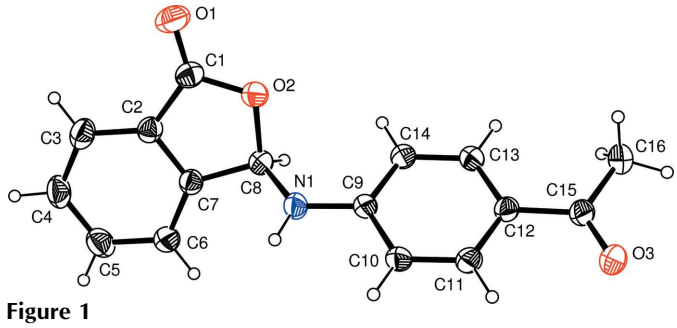


Figure 1
A view of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 30% probability level.

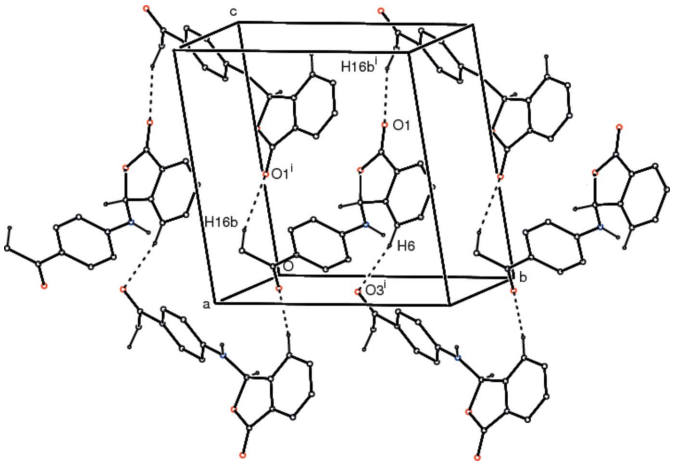


Figure 2
Part of the crystal structure of (I), showing the $R_4^4(33)$ hydrogen-bonded ring motifs, with hydrogen bonds drawn as dashed lines. For the sake of clarity, H atoms not involved in the motifs shown have been omitted. [Symmetry code: (i) $-x, y-\frac{1}{2}, 1-z$.]

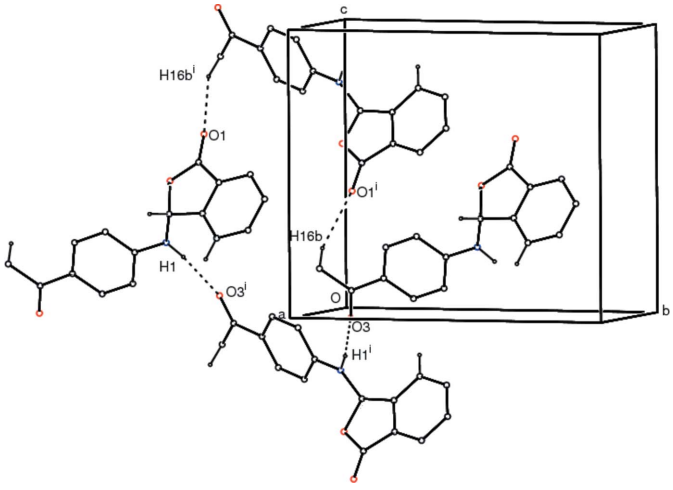


Figure 3
Part of the crystal structure of (I), showing the $R_4^4(29)$ hydrogen-bonded ring motifs with hydrogen bonds drawn as dashed lines. For the sake of clarity, H atoms not involved in the motifs shown have been omitted. [Symmetry code: (i) $-x, y-\frac{1}{2}, 1-z$.]

Büyükgüngör, 2006*b*), 51.7 (2)° in 3-(2,6-dimethylanilino)isobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2006*c*), 58.35 (15) and 54.82 (15)° in 3-{4-[4-(3-oxo-1,3-dihydroisobenzofuran-1-ylamino)benzyl]phenylamino}-isobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2006*d*), 78.43 (15)° in 3-anilinoisobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2006*e*), 51.45 (8)° in 3-(2-hydroxy-5-nitroanilino)isobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2006*f*) and 67.78 (14)° in 3-(4-ethoxyanilino)isobenzofuran-1(3*H*)-one (Odabaşoğlu & Büyükgüngör, 2006*g*).

The crystal packing is stabilized by N—H···O and C—H···O intermolecular hydrogen bonds and a C8—H8···π interaction (Table 2). The intermolecular C16—H16*b*···O1 and C6—H6···O3 hydrogen bonds generate $R_4^4(33)$ (Fig. 2), and the C16—H16*b*···O1, C6—H6···O3 and N1—H1···O3 bonds form $R_4^4(29)$ (Fig. 3) ring motifs (Etter, 1990; Bernstein *et al.*, 1995). These hydrogen-bonded rings are linked *via* $C(3)$ chains (Fig. 4), generating a three-dimensional framework (Fig. 5).

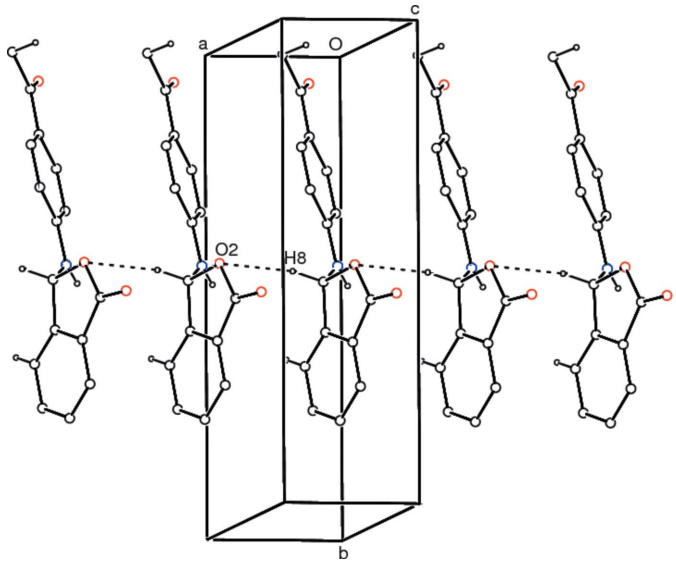


Figure 4
Part of the crystal structure of (I), showing the $C(3)$ chains with C8—H8···O2 hydrogen bonds drawn as dashed lines. For the sake of clarity, H atoms not involved in the motifs shown have been omitted.

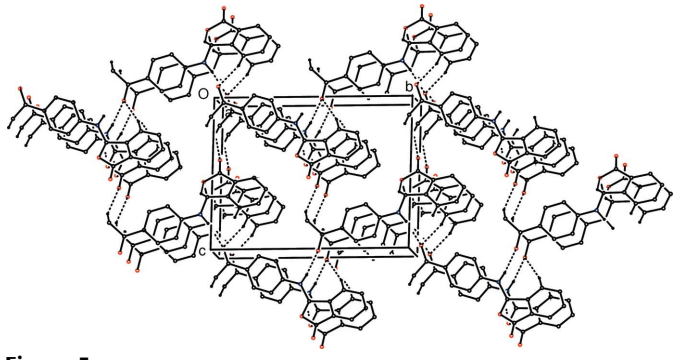


Figure 5
The packing diagram of (I), with hydrogen bonds drawn as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006*h*) using phthalaldehydic acid and 4-aminoactophenone as starting materials (yield 76%; m.p. 540–541 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

Crystal data

$C_{16}H_{13}NO_3$
$M_r = 267.27$
Monoclinic, $P2_1$
$a = 4.0243$ (5) Å
$b = 14.3117$ (12) Å
$c = 11.1107$ (12) Å
$\beta = 94.002$ (9)°
$V = 638.36$ (12) Å^3
$Z = 2$
$D_x = 1.391$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 296$ K
Prism, colorless
0.23 × 0.19 × 0.14 mm

Data collection

Stoe IPDS-2 diffractometer	1300 independent reflections
ω scans	1116 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{int} = 0.051$
7243 measured reflections	$\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2 + 0.0165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.071$	$\Delta\rho_{max} = 0.11$ e Å^{-3}
$S = 1.04$	$\Delta\rho_{min} = -0.12$ e Å^{-3}
1300 reflections	Extinction correction: *SHELXL97*
187 parameters	Extinction coefficient: 0.040 (6)
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.203 (3)	C9—N1	1.388 (3)
C1—O2	1.360 (3)	C12—C15	1.479 (3)
C2—C7	1.375 (3)	C15—O3	1.220 (3)
O1—C1—O2	121.2 (3)	N1—C8—O2	110.99 (18)
O1—C1—C2	130.2 (2)		
C11—C12—C15—O3	0.3 (3)	C13—C12—C15—C16	−0.3 (4)

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

*Cg*1 is the centroid of the C1/C2/C7/C8/O2 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.87 (3)	2.09 (3)	2.959 (3)	172 (3)
C6—H6···O3^{ii}	0.93	2.45	3.351 (3)	164
C8—H8···O2^{iii}	0.98	2.58	3.493 (3)	155
C16—H16*B*···O1^{iv}	0.96	2.57	3.457 (4)	154
C8—H8···*Cg*1^{iii}	0.98	2.87	3.671 (3)	140

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

All H atoms attached to C atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic [U_{iso}(H) = 1.2U_{eq}(C)] and C—H = 0.96 Å for methyl [U_{iso}(H) = 1.5U_{eq}(C)]. The H atom of the amino group was located in a Fourier difference map and freely refined. In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

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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