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3-Anilinoisobenzofuran-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 = 0.035
wR factor = 0.084
Data-to-parameter ratio = 13.4

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

Crystals of the title compound, $C_{14}H_{11}NO_2$, are stabilized by an intermolecular N—H···O hydrogen bond and a weak π–π interaction. N—H···O hydrogen-bond interactions generate *C*(6) chains. The phthalide section of the molecule is planar and the dihedral angle between the phthalide group and the benzene ring is 78.43 (5)°.

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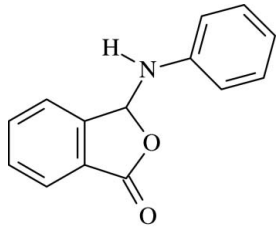
3-Substituted phthalides, Part IX.

Comment

The present work is part of a structural study of compounds of 3-phenylsubstituted phthalides (Odabaşoğlu, & Büyükgüngör, 2006*a*,*b*,*c*,*d*; Büyükgüngör & Odabaşoğlu, 2006) and we report here the structure of 3-anilinoisobenzofuran-1(3*H*)-one, (I).



(I)

The phthalide group (C1–C8/O2) is essentially planar, the largest deviation from the mean plane being 0.036 (5) Å for atom C4 (Fig. 1). The dihedral angle between the mean planes of the phthalide group and the phenyl ring is 78.43 (5)°.

The crystal packing is stabilized by intermolecular N—H···O hydrogen bonds, which generate *C*(6) chains (Etter, 1990) (Table 1). There are also weak π–π interactions which occur between the C2–C7 six-membered ring and its symmetry-related counterpart at $(1-x, 1-y, 1-z)$, with a centroid-to-centroid distance of 3.646 Å and a plane-to-plane separation of 3.541 Å.

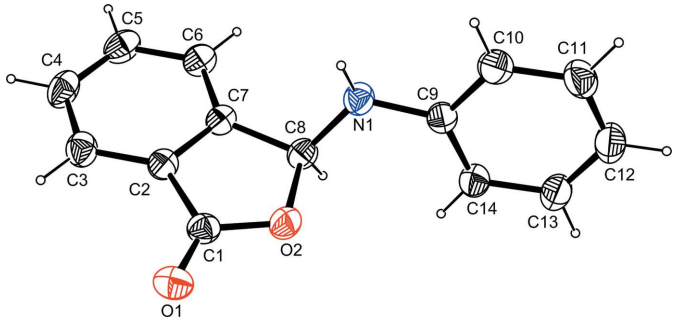


Figure 1
A view of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006*a*) using phthaldehydic acid and aniline as starting materials (yield 82%; m.p. 452–453 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a dimethylformamide solution at room temperature.

Crystal data

$C_{14}H_{11}NO_2$
M_r = 225.24
Monoclinic, $P2_1/c$
a = 12.5710 (14) Å
b = 7.0258 (6) Å
c = 15.7581 (15) Å
β = 128.525 (6)°
V = 1088.8 (2) Å^3
Z = 4
D_x = 1.374 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
Plate, light brown
0.38 × 0.25 × 0.07 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.969, T_{max} = 0.993
7405 measured reflections
2109 independent reflections
1457 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.084
S = 1.01
2109 reflections
157 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.043P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.13 e Å^{-3}
$\Delta\rho_{min}$ = −0.10 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.880 (18)	2.169 (18)	3.0117 (17)	160.2 (14)

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

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_{iso}(H) = 1.2U_{eq}(C). The H atom of the amino group was located in a Fourier difference map and freely refined with U_{iso}(H) = 1.2U_{eq}(N)

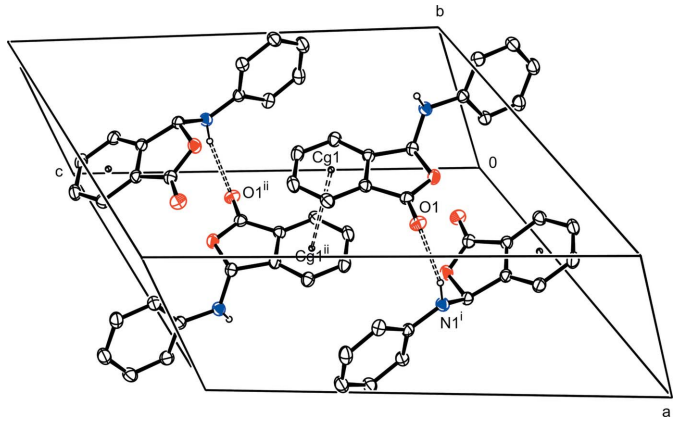


Figure 2
A packing diagram for (I), showing the N—H···O and π–π interactions represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. *Cg*1 is the centroid of the phthalide benzene ring. [Symmetry codes: (i) $-x+1, y-\frac{1}{2}, \frac{1}{2}-z$; (ii) $1-x, 1-y, 1-z$.]

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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