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

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3-Substituted phthalides, Part XXI.

Key indicators

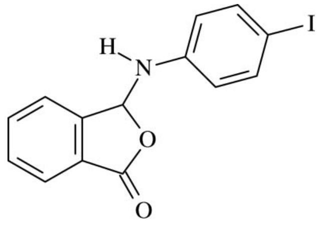
Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.016 Å
R factor = 0.063
wR factor = 0.245
Data-to-parameter ratio = 18.3

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

Crystals of the title compound, $C_{14}H_{10}INO_2$, whose asymmetric unit contains three independent molecules, are stabilized by three N—H···O, three C—H···O and one N—H···I intermolecular hydrogen bonds. In the structure, the N—H···O and C—H···O hydrogen bond interactions generate an edge-fused $R_2^2(11)$ ring motif which appears as a molecular ladder in the structure.

Comment

As part of a continuing study of the interplay between molecular conformation and supramolecular aggregation in 3-substituted phthalides (Büyükgüngör & Odabaşoğlu, 2006*a*,*b*; Odabaşoğlu & Büyükgüngör, 2006*a*,*b*,*c*,*d*,*e*,*f*,*g*,*h*,*i*,*j*,*k*,*l*,*m*,*n*,*o*,*p*,*q*,*r*, 2007), we now report the structure of 3-(4-iodoanilino)isobenzofuran-1(3*H*)-one, (I), which exhibits a supramolecular arrangement in the form of hydrogen-bonded molecular ladders (Fig. 2).



(I)

There are three symmetry-independent molecules in the asymmetric unit (Fig. 1). The dihedral angle between the *p*-iodophenyl rings and the mean planes of the phthalide groups are 76.1 (4), 86.5 (5) and 78.9 (5)°, comparable to the values of 75.58 (15)° in 3-(4-chloroanilino)phthalide (Büyükgüngör & Odabaşoğlu, 2006*a*), 74.10 (9)° in 3-(4-fluoroanilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*n*) and 62.2 (2)° in 3-(4-bromoanilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*o*).

The phthalide groups [C1–C8/O2, C15–C22/O3 and C29–C36/O5] are essentially planar, the largest deviations from the mean planes being 0.039 (10), 0.084 (10) and 0.062 (10) Å for atoms C4, C22 and C36, respectively. In (I), the crystal packing is stabilized by N—H···O, C—H···O and N—H···I intermolecular hydrogen bonds (Fig. 2, Table 1), with N—H···O and C—H···O hydrogen bonds generating an edge-fused $R_2^2(11)$ ring motif (Etter, 1990). The $R_2^2(11)$ rings appear as molecular ladders and I1 atoms are linked to H3a atoms. While the chloro and fluoro analogues of the title compound have π–π stacking interactions, (I) exhibits no such interaction, like its bromo analogue.

Experimental

Compound (I) was prepared as described by Odabaşoğlu & Büyükgüngör (2006*a*), using phthalaldehydic acid and 4-iodoaniline as starting materials (yield 85%, m.p. 452–453 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

Crystal data

$C_{14}H_{10}INO_2$
$M_r = 351.13$
Monoclinic, $P2_1/c$
$a = 24.017\ (3)$ Å
$b = 6.9536\ (6)$ Å
$c = 26.924\ (5)$ Å
$\beta = 120.207\ (11)^\circ$
$V = 3885.9\ (10)$ Å^3
$Z = 12$
$D_x = 1.801$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 2.47$ mm^{-1}
$T = 296$ K
Plate, pale yellow
0.66 × 0.41 × 0.14 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.285$, $T_{\max} = 0.604$
51463 measured reflections
7599 independent reflections
2725 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.075$
$\theta_{\max} = 26.0^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.063$
$wR(F^2) = 0.245$
$S = 0.99$
7599 reflections
415 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1178P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 1.24$ e Å^{-3}
$\Delta\rho_{\min} = -0.59$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1$^{\rm i}$	0.86	2.54	3.040 (8)	118
N2—H2A···O6$^{\rm ii}$	0.86	2.56	3.093 (10)	121
N3—H3A···O4$^{\rm iii}$	0.86	2.61	3.116 (10)	119
N3—H3A···I1$^{\rm iv}$	0.86	3.26	4.003 (8)	147
C8—H8···O1$^{\rm v}$	0.98	2.56	3.344 (9)	136
C22—H22···O6$^{\rm iii}$	0.98	2.55	3.356 (11)	139
C36—H36···O4$^{\rm ii}$	0.98	2.52	3.313 (12)	138

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

All H atoms were treated as riding on their parent atoms, with C—H = 0.93 Å for aromatic H, C—H = 0.98 Å for methine H, N—H = 0.86 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(parent). The highest peak in the final difference map is located 0.81 Å from atom I2.

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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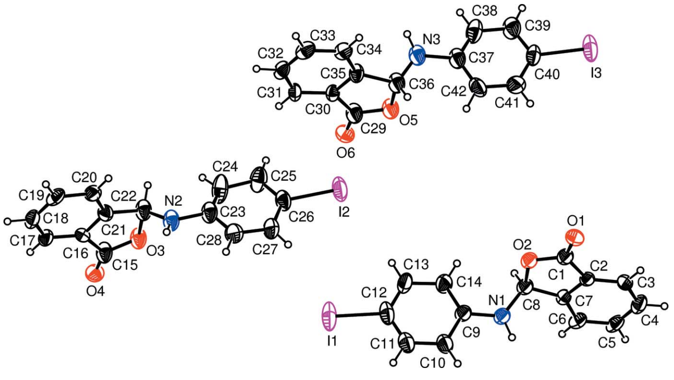

Figure 1
The asymmetric unit of (I) showing the atomic numbering scheme with displacement ellipsoids drawn at the 30% probability level.

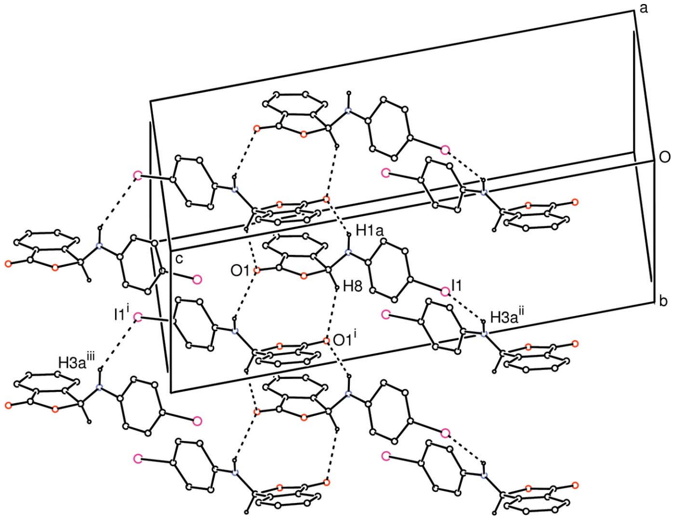

Figure 2
A partial packing diagram for (I), showing the N—H···O, C—H···O and N—H···I interactions represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $-x, y+\frac{1}{2}, \frac{3}{2}-z$; (ii) $x-1, y-\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x, -\frac{1}{2}+y, z+\frac{2}{3}$]

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