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3-[2-(Hydroxymethyl)anilino]isobenzofuran-1(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.035
wR factor = 0.092
Data-to-parameter ratio = 13.0

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, $C_{15}H_{13}NO_3$, is stabilized by inversion-related N—H···O, O—H···O and two C—H···O intermolecular hydrogen bonds. These hydrogen bonds generate edge-fused $R_2^1(7)$, $R_2^2(6)$, $R_2^1(7)$ and $R_4^4(28)$ ring motifs. The phthalide part of the molecule is planar and the dihedral angle between the phthalide group and the benzene ring is 68.76 (6)°.

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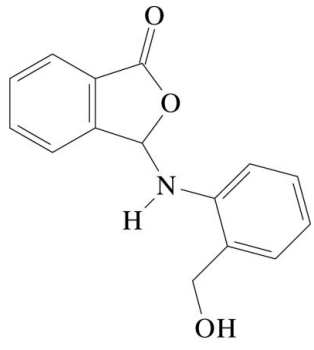
3-Substituted phthalides. Part XXV. Part XXIV: Odabaşoğlu & Büyükgüngör (2007).

Comment

As part of a continuing study of the interplay between molecular conformation and supramolecular aggregation in 3-substituted phthalides, we now report the structure of the title compound, 3-[2-(hydroxymethyl)phenylamino]isobenzofuran-1(3*H*)-one, (I) (Fig. 1).



(I)

The geometry of the molecule of (I) does not show any significant differences from the average geometry found for 3-anilinoisobenzofuran-1(3*H*)-ones (Odabaşoğlu & Büyükgüngör, 2006, 2007) (Table 1).

The phthalide group (C1–C8/O2) is planar, the largest deviation from the mean plane being 0.013 (1) Å for atom C1. The dihedral angle between the mean planes of the phthalide group and the phenyl ring is 68.76 (6)°.

The crystal packing of (I) is stabilized by inversion-related N—H···O, O—H···O and C—H···O intermolecular hydrogen bonds (Table 2). The C5—H5···O2^{iii} intermolecular hydrogen bonds generate *C*(7) chains. Parallel chains are linked *via* N—H···O, O—H···O and C—H···O hydrogen bonds and generate centrosymmetric $R_2^1(7)$, $R_2^2(6)$, $R_2^1(7)$ and $R_4^4(28)$ ring motifs (Fig. 2) (Etter, 1990).

Experimental

Compound (I) was prepared as described by Odabaşoğlu & Büyükgüngör (2007), using phthaldehydic acid and aminobenzyl alcohol as

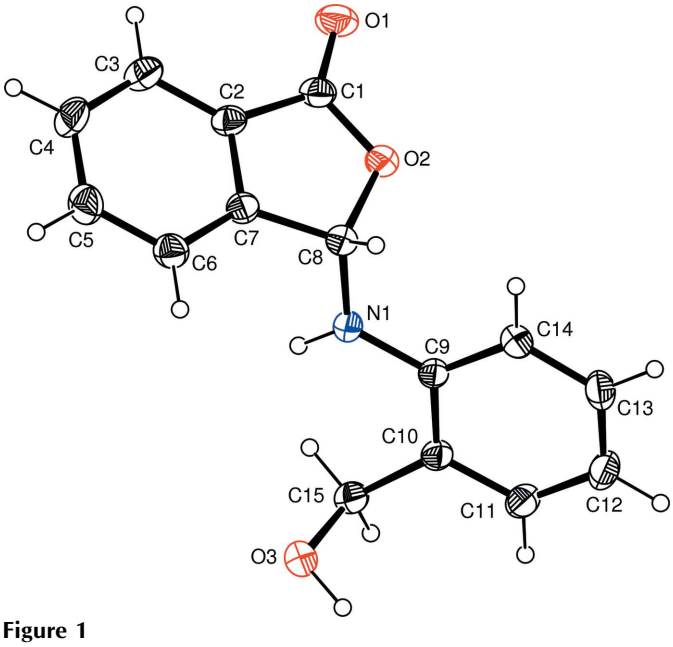


Figure 1
The molecular structure of (I), showing the atomic numbering scheme, with displacement ellipsoids drawn at the 30% probability level.

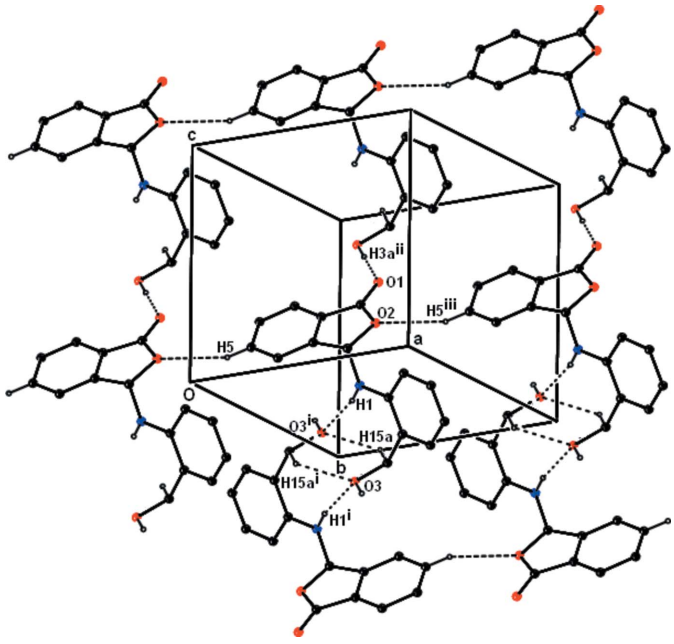


Figure 2
Part of the crystal structure of (I). For the sake of clarity, H atoms not involved in the hydrogen bonding motifs shown have been omitted. Hydrogen bonds are drawn as dashed lines. [Symmetry codes: (i) $-x$, $2-y$, $-z$; (ii) x, y, $z+1$; (iii) $x+1$,y, z].

starting materials (yield 95%; m.p. 426–427 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a solution in ethyl acetate at room temperature.

Crystal data

$C_{15}H_{13}NO_3$
$M_r = 255.26$
Triclinic, $P\overline{1}$
$a = 8.0032\ (12)$ Å
$b = 8.4448\ (13)$ Å
$c = 9.8464\ (14)$ Å
$\alpha = 83.926\ (12)^\circ$
$\beta = 87.035\ (12)^\circ$
$\gamma = 64.626\ (11)^\circ$
$V = 597.88\ (15)$ Å^3
$Z = 2$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm^{-1}
$T = 296$ K
0.66 × 0.44 × 0.20 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.951$, $T_{max} = 0.983$
10249 measured reflections
2340 independent reflections
2036 reflections with $I > 2\sigma(I)$
$R_{int} = 0.043$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.092$
$S = 1.03$
2340 reflections
180 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.2056 (16)	C2—C7	1.3785 (17)
C1—O2	1.3407 (16)	C9—N1	1.3953 (16)
O1—C1—O2	121.47 (13)	N1—C8—O2	111.53 (10)
O1—C1—C2	129.63 (13)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.859 (16)	2.205 (17)	3.0519 (16)	168.6 (14)
O3—H3A···O1^{ii}	0.95 (2)	1.91 (2)	2.8586 (16)	178.1 (19)
C5—H5···O2^{iii}	0.93	2.53	3.3949 (17)	155
C15—H15A···O3^{i}	0.97	2.48	3.2445 (18)	135

Symmetry codes: (i) $-x, -y+2, -z$; (ii) $x, y, z-1$; (iii) $x-1, y, z$.

All C-bound H atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic, 0.98 Å for methine and 0.97 Å for methylene H atoms, and with $U_{iso}(H) = 1.2U_{eq}(C)$. The N– and O-bound H atoms were located in a difference Fourier map and refined freely; refined O—H and N—H distances are in Table 2.

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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