Acta Crystallographica Section E
**Structure Reports**
**Online**
ISSN 1600-5368

# 3-(4-Ethoxyanilino)isobenzofuran-1(3*H*)-one

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The crystal structure of the title compound, $C_{16}H_{15}NO_3$, is stabilized by two N—H···O intermolecular hydrogen bonds and three C—H···$\pi$ interactions. N—H···O hydrogen bonds generate a $C_1^2(4)[R_1^2(4)]$ ring motif and the phthalide section of the molecule is planar. The dihedral angle between the phthalide group and the benzene ring is 67.78 (14)°.

Received 17 May 2006
Accepted 24 May 20063-
Substituted phthalides, Part *X*

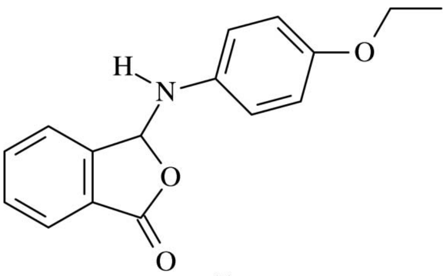
**Key indicators**

Single-crystal X-ray study
$T$ = 296 K
Mean $\sigma$(C–C) = 0.005 Å
$R$ factor = 0.040
$wR$ factor = 0.082
Data-to-parameter ratio = 8.1

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

## Comment

The present work is part of a structural study of compounds of 3-substituted phthalides (Odabaşoğlu & Büyükgüngör, 2006) and we report here the structure of 3-(4-ethoxyanilino)-isobenzofuran-1(3*H*)-one, (I) (Fig. 1 and Table 1).



(I)

The phthalide group (C1–C8,O2) is essentially planar, the largest deviation from the mean plane being 0.019 (4) Å for atom C4. The dihedral angle between the mean planes of the phthalide group and the benzene ring is 67.78 (14)°.

The crystal packing is stabilized by N—H···O intermolecular hydrogen bonds, which generate a $C_1^2(4)[R_1^2(4)]$ ring motif (Etter, 1990), and also by C—H···$\pi$ interactions (Table 2).

## Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006), using phthalaldehydic acid and 4-propylaniline as starting materials (yield 93%; m.p. 450–451 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.

*Crystal data*

$C_{16}H_{15}NO_3$
$M_r$ = 269.29
Orthorhombic, $Pna2_1$
$a$ = 8.6851 (11) Å
$b$ = 28.485 (3) Å
$c$ = 5.4644 (5) Å
$V$ = 1351.8 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.323 Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 K
Plate, colorless
0.39 × 0.22 × 0.04 mm

### *Data collection*

Stoe IPDS-2 diffractometer
$\omega$ scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{\min} = 0.974$, $T_{\max} = 0.996$
11317 measured reflections
1478 independent reflections
915 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.136$
$\theta_{\max} = 26.0°$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.082$
$S = 0.95$
1478 reflections
183 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0302P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.12$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.13$ e Å$^{-3}$
Extinction correction: *SHELXL97*
Extinction coefficient: 0.031 (4)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C1—O1 | 1.210 (4) | C8—N1 | 1.400 (4) |
| C1—O2 | 1.351 (4) | C9—N1 | 1.396 (4) |
| C2—C7 | 1.383 (4) | | |
| O1—C1—O2 | 120.8 (3) | N1—C8—O2 | 111.8 (2) |
| O1—C1—C2 | 130.0 (3) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1···O1$^{\rm i}$ | 0.86 | 2.46 | 3.263 (3) | 156 |
| N1—H1···O2$^{\rm i}$ | 0.86 | 2.54 | 3.309 (3) | 150 |
| C14—H14···*Cg*2$^{\rm ii}$ | 0.93 | 2.89 | 3.607 (4) | 135 |
| C15—H15*A*···*Cg*2$^{\rm iii}$ | 0.97 | 2.95 | 3.788 (4) | 146 |
| C16—H16*A*···*Cg*1$^{\rm iv}$ | 0.96 | 2.98 | 3.842 (4) | 150 |

Symmetry codes: (i) $x, y, z+1$; (ii) $-x, -y, z-\frac{1}{2}$; (iii) $-x+1, -y, z+\frac{1}{2}$; (iv) $-x, -y, z+\frac{1}{2}$. *Cg*1 and *Cg*2 are the centroids of the C2–C7 and C9–C13 rings, respectively.

In the absence of significant anomalous scattering effects, 1173 Friedel pairs were averaged. All H atoms were refined using a riding model, with C—H = 0.93 for aromatic, C—H = 0.98 Å for methine CH, N—H = 0.86 Å and C—H = 0.97 Å for methylene H atoms, with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$(C,N), and C—H = 0.96 Å and $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(C) for methyl H atoms.

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).

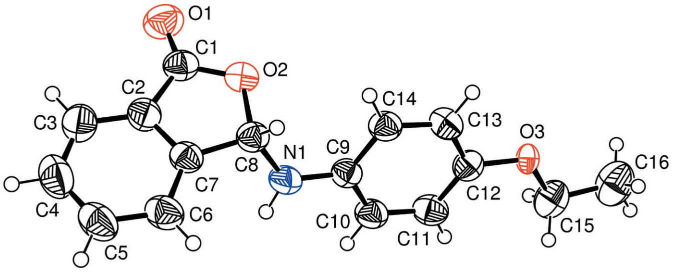


**Figure 1**
A view of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 50% probability level.

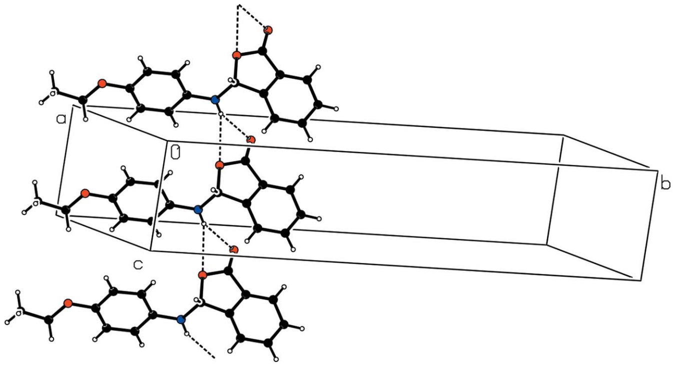


**Figure 2**
A partial packing diagram for (I), with hydrogen bonds shown as dashed lines.

The authors acknowledge the Faculty of Arts and Sciences, Ondokuz Mayıs University, Turkey, for the use of the Stoe IPDS II diffractometer (purchased under grant F.279 of the University Research Fund).

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