

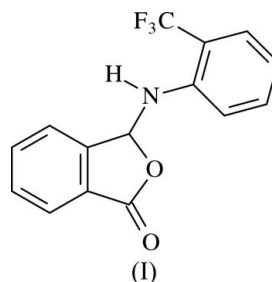
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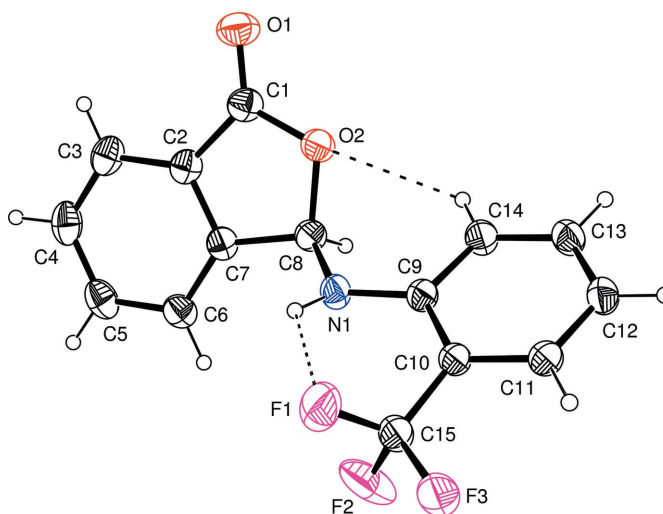
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ (C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.113
Data-to-parameter ratio = 12.6For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.3-[2-(Trifluoromethyl)anilino]isobenzofuran-1(3*H*)-oneThe crystal structure of the title compound, C₁₅H₁₀F₃NO₃, is stabilized by intramolecular N–H···F and C–H···O, and intermolecular N–H···O hydrogen bonds and by weak C–H··· π interactions. The N–H···O hydrogen bonds generate *C*(6) chains. The phthalide section of the molecule is planar, with a dihedral angle of 50.61 (8)° between the phthalide group and the benzene ring.Received 11 August 2006
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Part XVIII

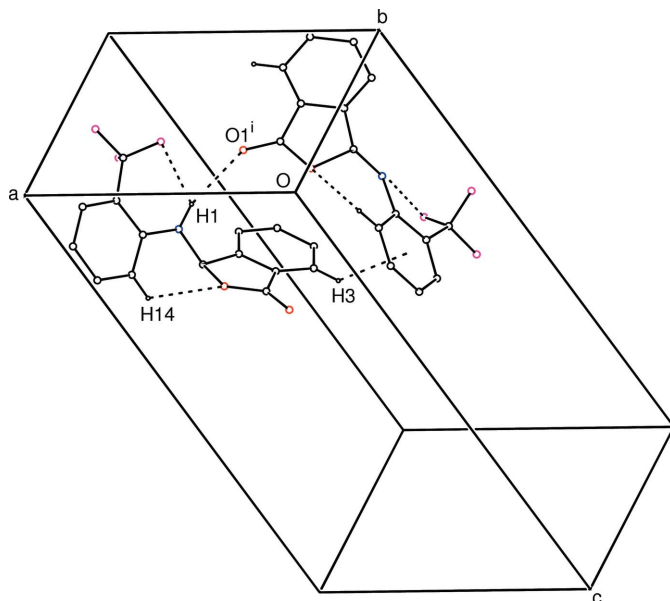
Comment

The present work is part of a structural study of compounds of 3-substituted phthalides and we report here the structure of 3-[2-(trifluoromethyl)anilino]isobenzofuran-1(3*H*)-one, (I) (Fig. 1 and Table 1).

Atom N1 atom in (I) is in an almost planar environment and the phthalide group (C1–C8/O2) is also essentially planar, the largest deviation from its mean plane being 0.055 (2) Å for

**Figure 1**

A view of (I), showing the atomic numbering scheme and displacement ellipsoids drawn at the 50% probability level. The hydrogen bonds are drawn as dashed lines.

**Figure 2**

Part of the crystal structure of (I), showing the formation of a hydrogen-bonded dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry code: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$.]

atom C8. The dihedral angle between the mean planes of the phthalide group and the trifluoromethylphenyl ring is $50.61(8)^\circ$. This angle was found to be $78.43(15)^\circ$ in 3-anilino-phthalide (Odabaşoğlu & Büyükgüngör, 2006a) and $54.55(10)^\circ$ in 3-(4-acetylanilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006b).

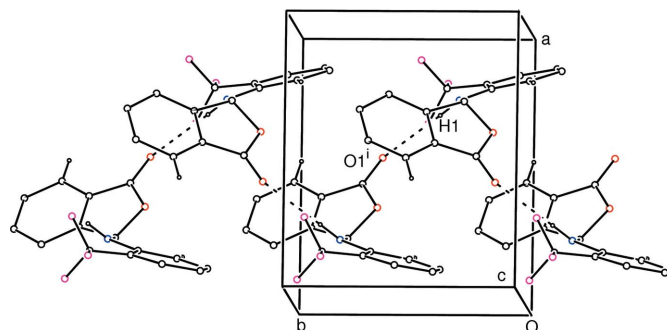
The crystal packing is stabilized by intramolecular N—H \cdots F and C—H \cdots O, and intermolecular N—H \cdots O hydrogen bonds and by weak C—H \cdots π interactions (Fig. 2). The intramolecular hydrogen bonds generate two *S*(6) rings (Figs. 1 and 2) and intermolecular N—H \cdots O hydrogen bonds generate *C*(6) chains (Fig. 3) (Etter, 1990); they are further linked through C3—H3 \cdots Cg1 interactions (Cg1 is the centroid of the C9—C14 ring). For the C3—H3 \cdots Cg1 contact (Fig. 2), the distances between atoms C3, H3 and the aromatic ring centroid are 3.530 (3) and 2.81 Å, respectively (symmetry code: $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; C3—H3 \cdots Cg1 = 136°).

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006c) using phthalaldehydic acid and 3-trifluoromethylaniline as starting materials (yield 75%; m.p. 405–407 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

Crystal data

$C_{15}H_{10}F_3NO_2$	$Z = 4$
$M_r = 293.24$	$D_x = 1.559 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 9.6389(9) \text{ \AA}$	$\mu = 0.13 \text{ mm}^{-1}$
$b = 7.7222(5) \text{ \AA}$	$T = 296 \text{ K}$
$c = 17.3829(15) \text{ \AA}$	Prism, colorless
$\beta = 105.072(7)^\circ$	$0.58 \times 0.31 \times 0.12 \text{ mm}$
$V = 1249.36(18) \text{ \AA}^3$	

**Figure 3**

A packing diagram for (I), showing the *C*(6) chains. N—H \cdots O hydrogen bonds are represented as dashed lines and H atoms not involved in hydrogen bonds have been omitted for clarity.

Data collection

Stoe IPDS-2 diffractometer	16157 measured reflections
ω scans	2462 independent reflections
Absorption correction: integration (<i>X-RED</i> ; Stoe & Cie, 2002)	1750 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.746, T_{\max} = 0.964$	$R_{\text{int}} = 0.081$
	$\theta_{\max} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2 + 0.2157P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.113$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.02$	$\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$
2462 reflections	$\Delta\rho_{\min} = -0.30 \text{ e \AA}^{-3}$
195 parameters	Extinction correction: <i>SHELXL97</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0105 (19)

Table 1

Selected geometric parameters (Å, °).

C1—O1	1.202 (2)	C2—C7	1.376 (3)
C1—O2	1.359 (2)	C9—N1	1.396 (2)
O1—C1—O2	121.63 (19)	N1—C8—O2	112.91 (15)
O1—C1—C2	130.2 (2)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1 \cdots F1	0.89 (2)	2.33 (2)	2.927 (2)	124.9 (18)
C14—H14 \cdots O2	0.93	2.46	2.994 (3)	117
N1—H1 \cdots O1 ⁱ	0.89 (2)	2.38 (2)	3.235 (2)	160.9 (19)

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

All C-bound H atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic and 0.98 Å for methine H atoms [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$]. Amino atom H1 atom was located in a difference Fourier map and refined with the N1—H1 distance restrained to 0.87 (2) Å.

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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