3-[3-(Trifluoromethyl)anilino]isobenzo-furan-1(3H)-one

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Crystals of the title compound, $C_{15}H_{10}F_3NO_3$, are stabilized by N—H···O and C—H···O intermolecular hydrogen bonds and by weak C—H···π interactions. In the structure, paired C—H···O hydrogen bonds link the molecules into $R_2^2(10)$ dimers. The hydrogen-bonded $R_2^2(10)$ dimers are linked by inter-molecular N—H···O hydrogen bonds and generate $R_6^4(22)$ rings. The phthalide section of the molecule is planar and the dihedral angle between the phthalide group and the benzene ring is 56.31 (17)°.
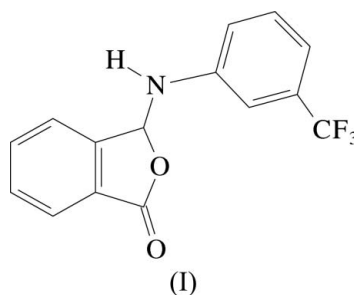
Comment

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

The phthalide group (atoms C1–C8/O2) is essentially planar, the largest deviation from the mean plane being 0.042 (3) Å for atom C8. The dihedral angle between the mean planes of the phthalide group and the trifluoromethylphenyl ring is 56.31 (17)°. This angle is 54.55 (10)° in 3-[2-(trifluoro-methyl)anilino]phthalide (Odabaşoğlu & Büyükgüngör, 2006a), 78.43 (15)° in 3-anilinophthalide (Odabaşoğlu &
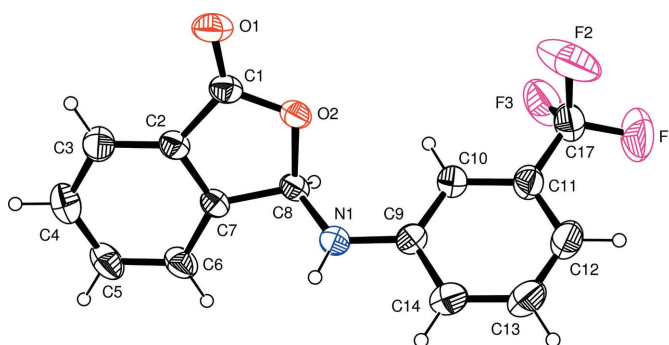
Figure 1
A view of (I), showing the atomic numbering scheme, with displacement ellipsoids drawn at the 30% probability level.
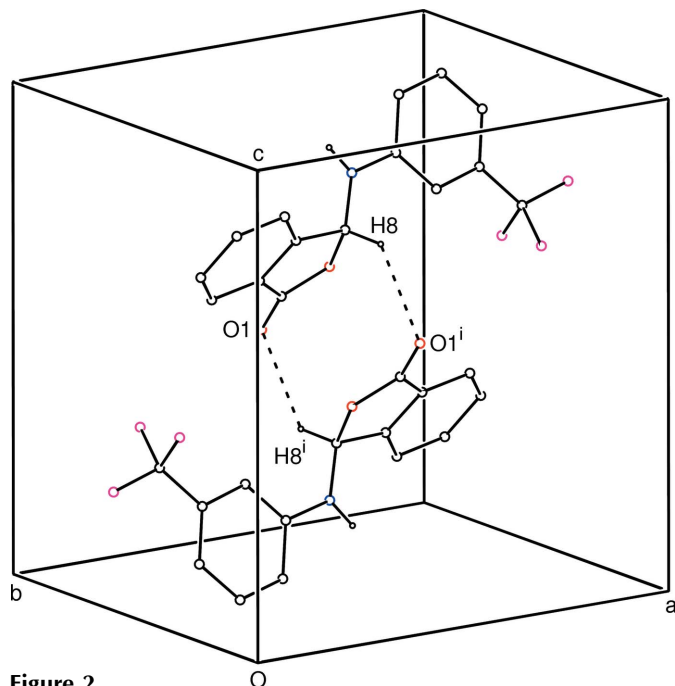
Figure 2
A packing diagram for (I). Dashed lines indicate hydrogen bonds.
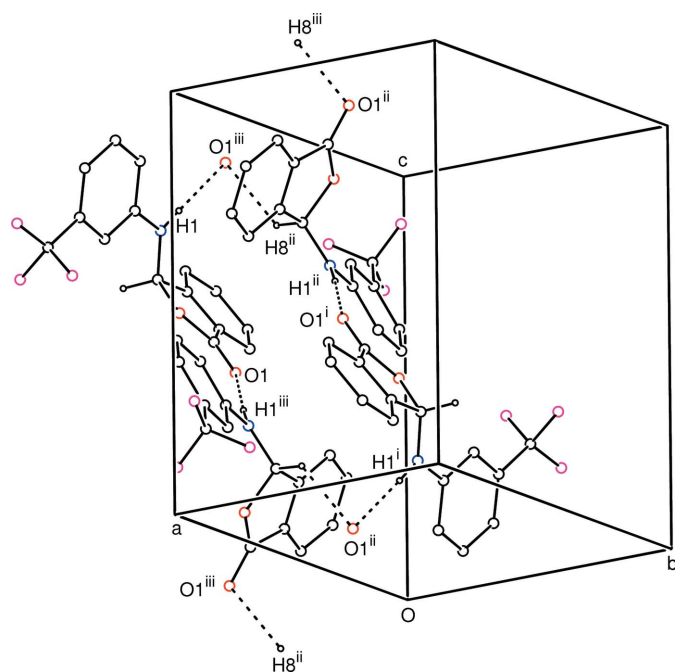

Figure 3
Part of the crystal structure of (I), with hydrogen bonds drawn as dashed lines, showing the formation of a hydrogen-bonded dimer. For the sake of clarity, H atoms bonded to C atoms have been omitted. [Symmetry code: (i) $1 - x, 1 - y, 1 - z$].

Büyükgüngör, 2006b), and 54.55 (10)° in 3-(4-acetyl-anilino)phthalide (Odabaşoğlu & Büyükgüngör, 2006c).

The crystal packing is stabilized by C—H···O and N—H···O intermolecular hydrogen bonds, which generate $R_2^2(10)$ (Fig. 2) and $R_6^4(22)$ rings (Fig. 3) (Etter, 1990), and also by C—H···π interactions (Fig. 4, Table 2).
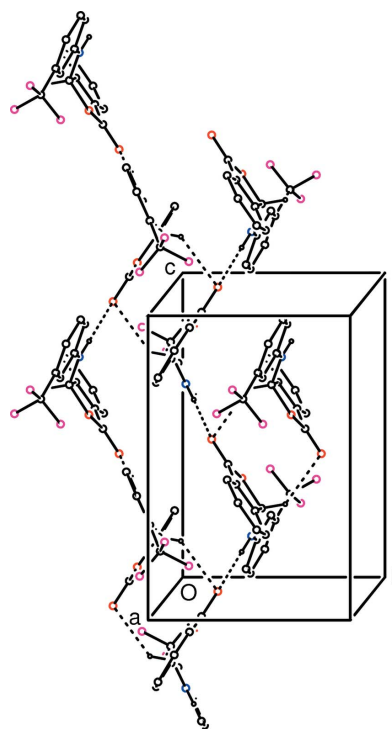

Figure 4
A packing diagram for (I), showing the $R_6^4(22)$, hydrogen bonds and C—H···π interactions represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $1 - x, 1 - y, z - \frac{1}{2}$; (iii) $x, y - 1, z + \frac{1}{2}$].

Experimental

The title compound, (I), was prepared as described by Odabaşoğlu & Büyükgüngör (2006d), using phthalaldehydic acid and 3-fluoro-methylaniline as starting materials (yield 78%; m.p. 417–418 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a glacial acetic acid solution at room temperature.

Crystal data

$C_{15}H_{10}F_3NO_2$	$Z = 4$
$M_r = 293.24$	$D_x = 1.454$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 13.4659\ (9)$ Å	$\mu = 0.13$ mm^{-1}
$b = 8.1794\ (7)$ Å	$T = 296$ K
$c = 12.2649\ (8)$ Å	Prism, colourless
$\beta = 97.400\ (5)°$	$0.61 \times 0.42 \times 0.12$ mm
$V = 1339.64\ (17)$ Å^3	

Data collection

Stoe IPDS-2 diffractometer	14507 measured reflections
ω scans	2629 independent reflections
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	1933 reflections with $I > 2\sigma(I)$
$T_{min} = 0.942$, $T_{max} = 0.986$	$R_{int} = 0.104$
	$\theta_{max} = 26.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.071$	$+ 1.3237P]$
$wR(F^2) = 0.198$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
2629 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
195 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	Extinction correction: SHELXL97
	Extinction coefficient: 0.011 (3)

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.203 (4)	C2—C3	1.372 (5)
C1—O2	1.344 (4)	C9—N1	1.393 (4)
O1—C1—O2	122.0 (3)	N1—C8—O2	111.5 (3)
O1—C1—C2	128.8 (3)		

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$O1[i]	0.83 (4)	2.14 (4)	2.962 (4)	176 (4)
C8—H8$\cdots$O1[ii]	0.98	2.52	3.264 (4)	133
C8—H8$\cdots$Cg1[iii]	0.98	3.31	3.979 (4)	128

Symmetry codes: (i) $x, -y + \frac{3}{2}, z + \frac{1}{2}$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$. Cg1 is the centroid of the five-membered ring

The NH group H atom (H1) was found in a difference Fourier map and refined freely. All other H atoms were refined using the riding-model approximation, with C—H = 0.93 for aromatic H atoms and C—H = 0.98 Å for methine H atoms [U_{iso}(H) = 1.2U_{eq}(C)].

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