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[2-Methyl-4-(3-oxo-1,3-dihydroisobenzofuran-1-ylamino)phenyl]isobenzofuran-1(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.009 Å
R factor = 0.061
wR factor = 0.184
Data-to-parameter ratio = 6.2

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, $C_{23}H_{17}NO_4$, is stabilized by intermolecular N—H···O and C—H···O hydrogen bonds and C—H···π interactions. The C—H···O hydrogen bonds link the molecules into ladders whose uprights form $C(7)$ chains and whose rungs enclose $R_2^2(28)$ rings. These motifs generate a three-dimensional network by N—H···O hydrogen bonds and C—H···π interactions. The phthalide ring systems of the molecule are almost planar and form dihedral angles of 64.1 (3) and 88.3 (3)° with the benzene ring.

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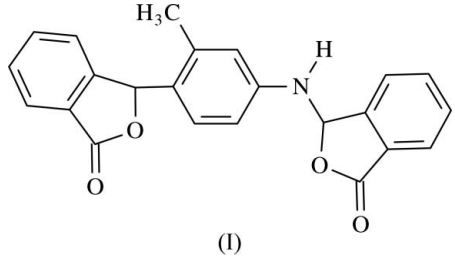
3-Substituted phthalides, Part XX.

Comment

The present work is part of a structural study of compounds of 3-substituted phthalides (Büyükgüngör & Odabaşoğlu, 2006*a*,*b*,*c*; Odabaşoğlu & Büyükgüngör, 2006*a*,*b*,*c*,*d*,*e*,*f*,*g*,*h*,*i*,*j*,*k*,*l*,*m*,*n*,*o*,*p*,*q*,*r*) and we report here the structure of the title compound, (I) (Fig. 1).



(I)

The phthalide groups (*A* = C1–C8/O2; *B* = C9–C14; *C* = C16–C23/O4) are essentially planar, with the largest deviations from the mean plane being 0.048 (6) and 0.020 (6) Å for atoms C8 and C17, respectively. The dihedral angles between the *A*/*B*, *A*/*C* and *B*/*C* planes are 64.1 (3), 55.2 (2) and 88.3 (3)°, respectively (Fig. 1).

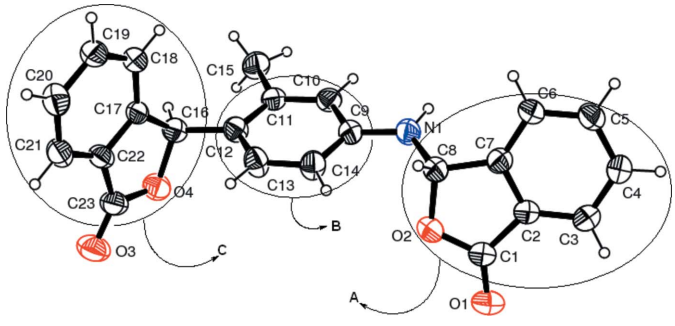


Figure 1
The molecular structure of (I), showing the atomic numbering scheme with displacement ellipsoids drawn at the 30% probability level.

The crystal packing is stabilized by one N—H···O and two C—H···O intermolecular hydrogen bonds and two C—H···π interactions (Table 1). The C—H···O hydrogen bonds link the molecules into ladders whose uprights form $C(7)$ chains (Fig. 2) and whose rungs enclose $R_2^2(28)$ rings (Etter, 1990). The molecular ladders generate a three-dimensional network by N—H···O hydrogen bonds and C—H···π interactions (Fig. 3).

Experimental

Compound (I) was prepared as described (Odabaşoğlu & Büyükgüngör, 2006*a*), using phthalaldehydic acid and 3-methylaniline as starting materials (yield 65%; m.p. 405–406 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of a DMF solution at room temperature.

Crystal data

$C_{23}H_{17}NO_4$
M_r = 371.38
Monoclinic, *Pc*
a = 5.1039 (3) Å
b = 6.1761 (6) Å
c = 28.5758 (18) Å
β = 92.444 (5)°
V = 899.95 (12) Å^3
Z = 2
D_x = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
Prism, light brown
0.54 × 0.30 × 0.12 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.963, T_{max} = 0.990
8708 measured reflections
1592 independent reflections
1251 reflections with $I > 2\sigma(I)$
R_{int} = 0.102
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.185
S = 1.09
1592 reflections
258 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1066P)^2 + 0.2251P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.055 (13)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86 (7)	2.26 (6)	3.118 (7)	164 (7)
C5—H5···O1^{ii}	0.93	2.62	3.256 (9)	126
C19—H19···O3^{ii}	0.93	2.44	3.147 (9)	133
C15—H15b···$Cg1^{iii}$	0.96	3.00	3.861 (8)	150
C4—H4···$Cg2^{iv}$	0.93	3.18	3.912 (9)	137

Symmetry codes: (i) $x, y+1, z$; (ii) $x-1, y+1, z$; (iii) $x+1, y, z$; (iv) $x-1, -y+1, z+\frac{1}{2}$. *Cg*1 and *Cg*2 are the centroids of the C9–C14 and C17–C22 rings, respectively

All H atoms attached to C atoms were treated as riding on their parent atoms, with C—H = 0.93 Å for aromatic H, 0.98 Å for methine H and 0.96 Å for methyl H, with U_{iso}(H) = 1.2U_{eq}(C). The H atom of the amino group was located in a Fourier difference map and freely refined, with U_{iso}(H) = 1.2U_{eq}(N). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

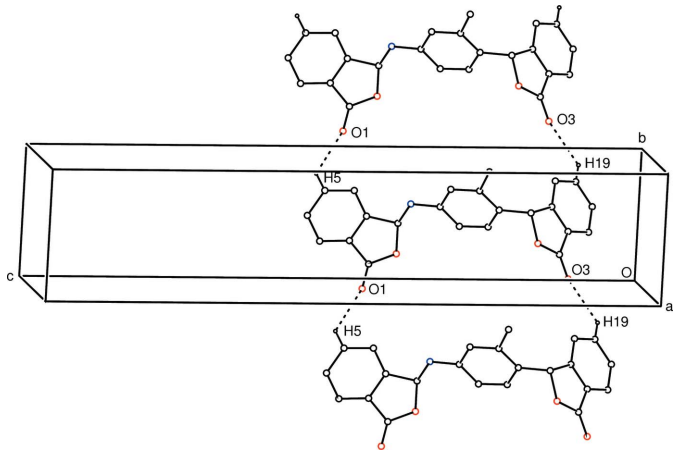


Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded molecular ladder and $R_2^2(28)$ rings. H atoms not involved in hydrogen bonds have been omitted for clarity.

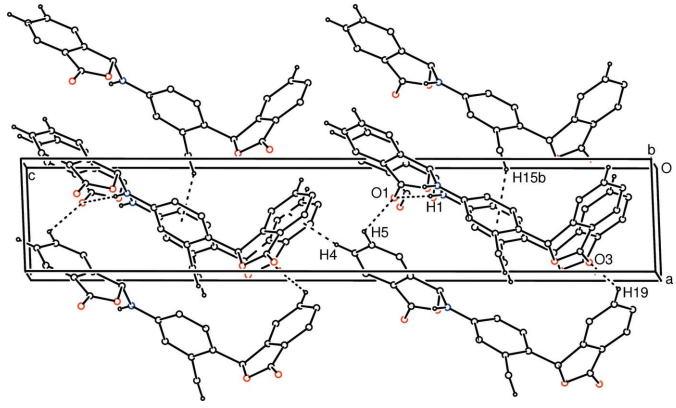


Figure 3
A packing diagram for (I), showing the N—H···O, C—H···O and C—H···π interactions represented as dashed lines. H atoms not involved in hydrogen bonds have been omitted for clarity.

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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