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3-(4-Methylpyridin-2-ylamino)isobenzofuran-1(3*H*)-one

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.006 Å
R factor = 0.079
wR factor = 0.237
Data-to-parameter ratio = 15.0

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

Crystals of the title compound, $C_{14}H_{12}O_2N_2$, are stabilized by inversion-related N—H···N and C—H···O intermolecular hydrogen bonds and also by two C—H···π interactions. The N—H···N and C—H···O hydrogen bonds generate $R_2^2(8)$ and $R_2^2(10)$ ring motifs, respectively, and the phthalide section of the molecule is planar. The dihedral angle between the phthalide group and the pyridyl ring is 82.06 (17)°.

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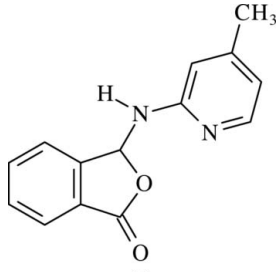
3-Substituted phthalides, Part VII

Comment

In separate papers, we have reported the syntheses and crystal structures of 3-(2-pyridylamino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*a*) and 3-(3-pyridylamino)phthalide (Odabaşoğlu & Büyükgüngör, 2006*b*). We report here the structure of 3-(4-methylpyridin-2-ylamino)isobenzofuran-1(3*H*)-one (Fig. 1 and Table 1).



(I)

The phthalide group (C1–C8/O2) is planar, the largest deviation from the mean plane being 0.040 (4) Å for atom C8. The dihedral angle between the mean planes of the phthalide group and the pyridyl ring is 82.06 (17)°.

The crystal packing is stabilized by inversion-related N1—H1···N2^{i} and C8—H8···O1^{ii} intermolecular hydrogen bonds,

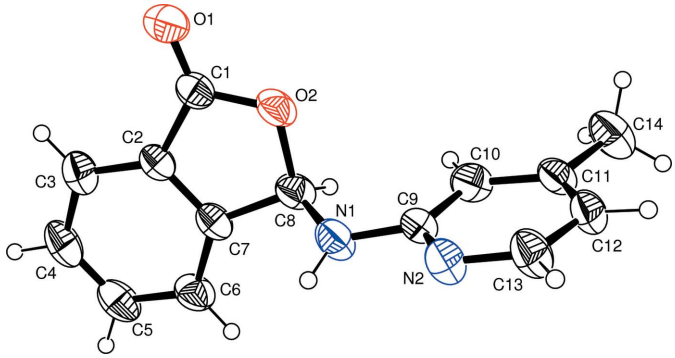


Figure 1
A view of (I), showing the atomic numbering scheme, with displacement ellipsoids drawn at the 40% probability level.

which generate centrosymmetric $R_2^2(8)$ and $R_2^2(10)$ ring motifs, respectively (Etter, 1990), and C—H···π interactions (Fig. 2 and Table 2).

Experimental

The title compound was prepared as described by Odabaşoğlu & Büyükgüngör (2006*c*), using phthalaldehydic acid and 2-amino-4-methylpyridine as starting materials (yield 92%, m.p. 435–437 K). Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an ethanol (95%) solution at room temperature.

Crystal data

$C_{14}H_{12}N_2O_2$
M_r = 240.26
Triclinic, $P\overline{1}$
a = 7.6621 (18) Å
b = 8.0381 (18) Å
c = 10.616 (2) Å
α = 87.387 (17)°
β = 78.177 (18)°
γ = 78.456 (18)°
V = 627.0 (2) Å^3
Z = 2
D_x = 1.273 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 296 K
Prism, colorless
0.47 × 0.36 × 0.17 mm

Data collection

Stoe IPDS-2 diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.960, T_{max} = 0.987
5736 measured reflections
2454 independent reflections
1575 reflections with $I > 2\sigma(I)$
R_{int} = 0.079
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.080
$wR(F^2)$ = 0.237
S = 1.09
2454 reflections
164 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0967P)^2 + 0.443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.209 (5)	C7—C8	1.517 (5)
C1—O2	1.369 (5)	C8—N1	1.403 (5)
C2—C7	1.381 (5)	C9—N1	1.406 (5)
O1—C1—O2	121.5 (3)	N1—C8—O2	111.0 (3)
O1—C1—C2	130.5 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···N2^{i}	0.86	2.31	3.075 (5)	149
C8—H8···O1^{ii}	0.98	2.43	3.211 (6)	136
C6—H6···*Cg*1^{iii}	0.93	3.37	4.039 (4)	131
C13—H13···*Cg*2^{i}	0.93	2.82	3.702 (5)	160

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

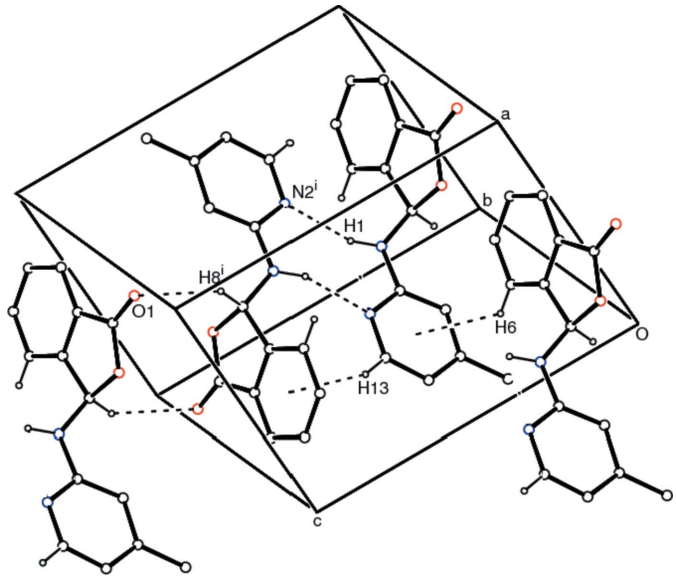


Figure 2
A packing diagram for (I), with hydrogen bonds and C—H···π interactions drawn as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

All H atoms were refined using the riding-model approximation, with C—H = 0.93 Å for aromatic, 0.98 Å for methine and N—H = 0.86 Å for amino H atoms, with U_{iso}(H) = 1.2U_{eq}(parent atom), and C—H = 0.96 Å for methyl H atoms with U_{iso}(H) = 1.5U_{eq}(C).

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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