Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-(3-Amino-1-benzofuran-2-yl)-2-mesitylethanone

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Received 7 April 2004
Accepted 11 June 2004
Online 19 June 2004

The title compound, $C_{19}H_{19}NO_2$, features a benzofuran ring system coplanar with an amino substituent and linked to a mesityl group by an acetyl bridge. In the crystal structure, symmetry-related molecules are linked by N—H···O intermolecular hydrogen bonds involving one amino H atom and the O atom of the acetyl group to form infinite chains. The other amino H atom is involved in an intramolecular hydrogen bond with the acetyl O atom.

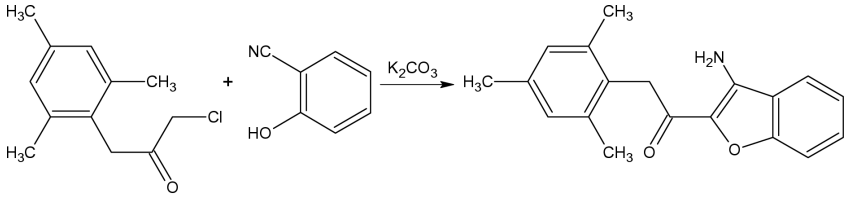
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.054
wR factor = 0.132
Data-to-parameter ratio = 11.9

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

Comment

Benzofuran derivatives possess antimicrobial, bacteriostatic, bactericidal, fungistatic and fungicidal activities (Hassaneen *et al.*, 2002). Moreover, benzofurans are building blocks for optical brighteners and are applied, for example, in combination with benzimidazoles as biphenyl end groups (Schmidt, 1999). Many of the natural benzofurans have physiological, pharmacological and toxic properties and, as a result, there is continuing interest in their chemical synthesis (Kappe *et al.*, 1997).



(1) (2)

The benzofuran ring system of the title compound, (2), is planar [with a maximum deviation from the plane of 0.101 (3) Å for C7] and the acetyl group is slightly twisted about the C1—C9 bond, as seen from the torsion angles O1—C1—C9—O2 [5.7 (3)°] and C2—C1—C9—C10 [13.2 (3)°]. Because of the amino group, the acetyl group is more twisted about the C1—C9 bond than in a similar compound (Arıcı *et al.*, 2004). The benzofuran ring system is linked to the mesityl group by the acetyl group. The dihedral angle between the benzofuran ring system and the mesityl group is 79.91 (9)°.

The structure is stabilized by intramolecular and intermolecular hydrogen-bonding interactions. In the crystal structure, molecules related by the 2_1 rotation axis are linked by N—H···O intermolecular hydrogen bonds involving an amino H atom and the O atom of the acetyl group to form infinite chains along the b axis. The other amino H atom is involved in an intramolecular hydrogen bond with the acetyl O atom. Adjacent chains are interlinked through weak C—H···π interactions involving the furan ring.

Experimental

A mixture of 1-chloro-3-mesitylacetone, (1) (5 g, 23.73 mmol), 2-hydroxybenzaldehyde (2.85 g, 24 mmol) and K_2CO_3 (6.55 g, 47.46 mmol) in absolute acetone was refluxed for 8 h. After cooling, compound (2) (6.02 g, 89.3%) was filtered off, washed with water, dried and recrystallized from tetrahydrofuran.

Crystal data

$C_{19}H_{19}NO_2$
M_r = 293.35
Monoclinic, $P2_1/c$
a = 10.3779 (12) Å
b = 10.3151 (11) Å
c = 15.2789 (13) Å
β = 105.116 (4)°
V = 1579.0 (3) Å^3
Z = 4
D_x = 1.234 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2.4–24.6°
μ = 0.08 mm^{-1}
T = 293 (2) K
Prism, colourless
0.25 × 0.20 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (Fair, 1990)
T_{min} = 0.981, T_{max} = 0.988
2499 measured reflections
2370 independent reflections
1392 reflections with $I > 2\sigma(I)$
R_{int} = 0.046
θ_{max} = 24.6°
$h = -12 \rightarrow 0$
$k = -12 \rightarrow 0$
$l = -17 \rightarrow 17$
3 standard reflections
frequency: 120 min
intensity decay: 0.7%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.132
S = 1.01
2370 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0639P)^2 + 1.0373P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.097 (19)

Table 1
Selected bond distances (Å).

C1—O1	1.408 (4)	C4—O1	1.373 (4)
C2—N1	1.346 (4)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2	0.86	2.37	2.927 (4)	122
N1—H1B···O2^{i}	0.86	2.43	3.076 (4)	133

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

All H atoms were positioned geometrically (N—H = 0.86 and C—H = 0.93–0.97 Å)and refined as riding, with U_{eq}(H) = 1.2U_{eq}(C,N).

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1993); cell refinement: *CAD*-4 *EXPRESS*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*2000 (Spek, 2000); software used to prepare material for publication: *SHELXL*97.

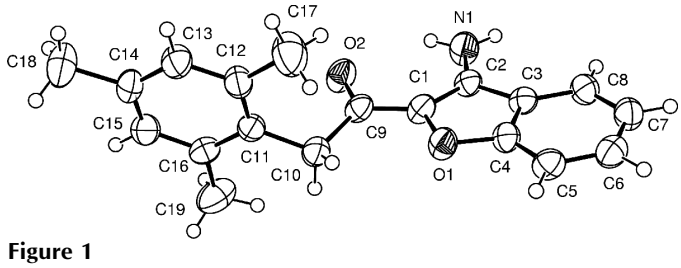


Figure 1
A view of the title compound with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small circles with arbitrary radii.

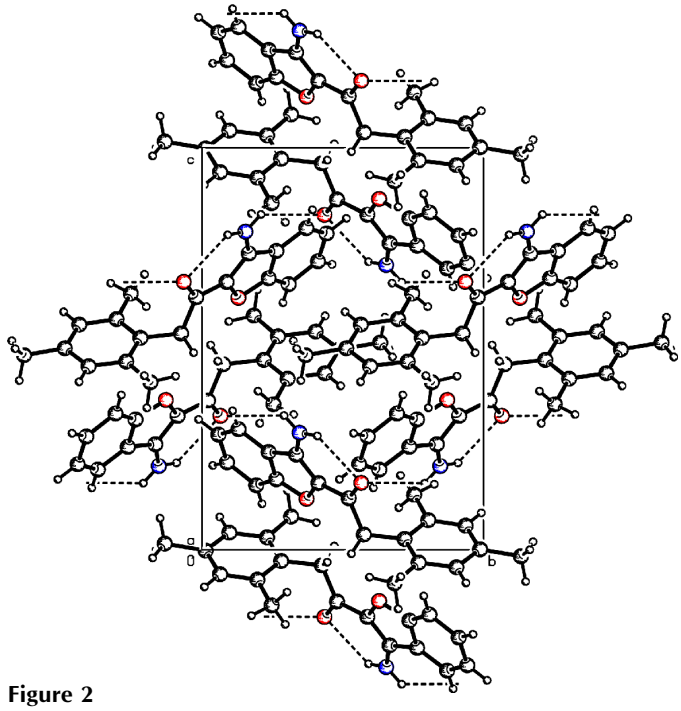


Figure 2
A view of the packing in (2), showing the intermolecular and intramolecular interactions.

The authors acknowledge the purchase of the CAD-4 diffractometer under grant DPT/TBAG1 from the Scientific and Technical Research Council of Turkey.

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