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1-(1-Benzofuran-2-yl)-2-mesitylethanone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.058
wR factor = 0.154
Data-to-parameter ratio = 12.9

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

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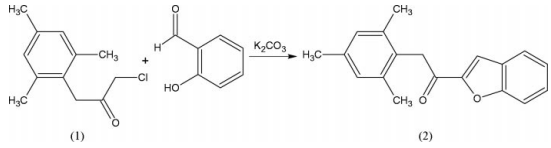
The benzofuran ring system in the title compound, $C_{19}H_{18}O_2$, is planar and is linked to the mesityl group *via* an acetyl group. In the crystal structure, symmetry-related molecules are connected to form chains by C—H···O intermolecular hydrogen bonds.

Comment

Benzofuran derivatives are nowadays an important class of organic compounds that occur in a great number of natural products. They are used in cosmetics and as synthetic pharmaceuticals (Bogdal & Warzala, 2000). 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).



The benzofuran ring system in the title compound, (2), is planar, with a maximum deviation from the plane of 0.0257 (3) Å for C8 (Fig. 1). The acetyl group is slightly twisted about the C8—C9 bond, as seen from the torsion angles O1—C8—C9—O2 = 1.7 (3)° and C7—C8—C9—C10 = 0.6 (3)°. The mesityl group is also planar and the dihedral angle between the benzofuran ring system and the mesityl group is 89.08 (4)°.

The structure is stabilized by van der Waals interactions and symmetry-related molecules are linked to form chains *via* C—H···O intermolecular hydrogen bonds (Table 2).

Experimental

A mixture of 1-chloro-3-mesitylacetone, (1) (5 g, 23.73 mmol), 2-hydroxybenzaldehyde (2.93 g, 24 mmol) and K_2CO_3 (4.91 g,

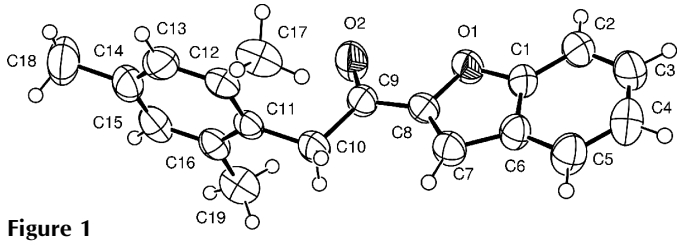


Figure 1
An *ORTEP*-3 (Farrugia, 1997) drawing of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small circles of arbitrary radii.

35.59 mmol) in 200 ml absolute acetone was refluxed for 5 h. After cooling, 1-(1-benzofuran-2-yl)-2-mesitylethanone, (2) (5.8 g, 87.8%) was filtered off, washed with water, dried and recrystallized from aqueous ethanol (95%) to yield colourless crystals.

Crystal data

$C_{19}H_{18}O_2$
M_r = 278.33
Monoclinic, $P2_1/c$
a = 8.133 (5) Å
b = 15.762 (5) Å
c = 11.752 (5) Å
β = 95.231 (5)°
V = 1500.2 (12) Å^3
Z = 4
D_x = 1.232 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 2.6–25.7°
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 (*MolEN*; Fair, 1990)
T_{min} = 0.973, T_{max} = 0.980
2570 measured reflections
2467 independent reflections
1330 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.7°
$h = -9 \rightarrow 9$
$k = -19 \rightarrow 0$
$l = -14 \rightarrow 0$
3 standard reflections
frequency: 120 min
intensity decay: 0.7%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.154
S = 1.02
2467 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0891P)^2 + 0.3519P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.012 (3)

Table 1
Selected geometric parameters (Å, °).

C1—O1	1.379 (4)	C9—O2	1.210 (4)
C8—O1	1.389 (4)		
O1—C1—C2	124.9 (3)	O2—C9—C8	121.6 (3)
O1—C1—C6	110.4 (3)	O2—C9—C10	122.7 (3)
O1—C8—C9	116.0 (3)	C1—O1—C8	105.9 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.93	2.52	3.432 (5)	165

Symmetry code: (i) $-x, -y, 2-z$.

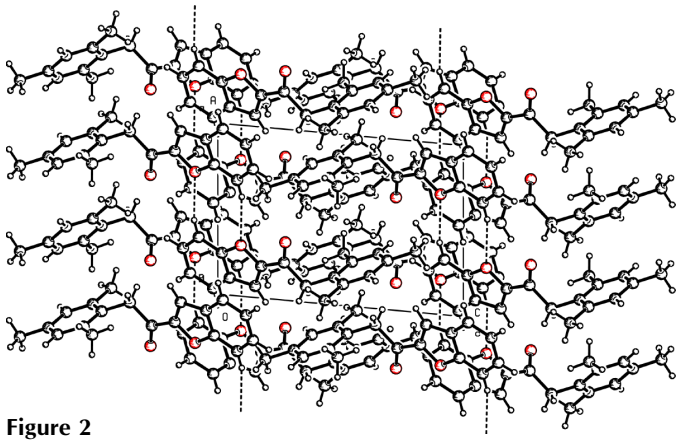


Figure 2
A packing diagram of the crystal structure. The dashed lines indicate hydrogen bonds.

H atoms were positioned geometrically, with C—H in the range 0.93–0.97 Å. They were refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *CAD*-4 *EXPRESS* (Enraf–Nonius, 1993); cell refinement: *CAD*-4 *EXPRESS*; data reduction: *XCAD*4 (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97; molecular graphics: *PLATON* (Spek, 2000); software used to prepare material for publication: *SHELXL*97.

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