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1-(1-Benzofuran-2-yl)ethanone *O*-(2-chlorobenzoyl)oxime

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
Disorder in main residue
R factor = 0.032
wR factor = 0.078
Data-to-parameter ratio = 14.4

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

The title compound, $C_{17}H_{12}ClNO_3$, displays the characteristic features of benzofuran derivatives. The molecule is not planar. Intermolecular C—H···O interactions help to stabilize the structure.

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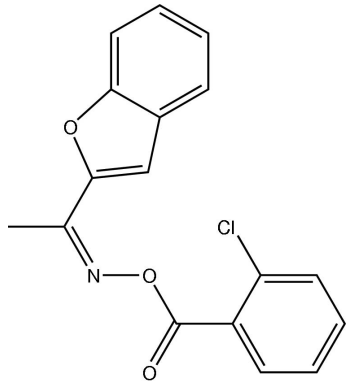
Comment

Oxime derivatives are bioactive compounds. It has been reported that free oximes and their ethers or esters show notably high activities (Massolini *et al.*, 1994; Demirayak *et al.*, 2002) when used as medicines and pesticides. In asymmetric synthesis, these compounds are good precursors for chiral amines. In most cases, they are synthesized in two steps, *viz.* condensation between a carbonyl compound and hydroxylamine followed by alkylation with an alkyl halide in the presence of a base under phase-transfer catalytic (PTC) conditions. These compounds have also been prepared by condensation of alkyl hydroxylamines with carbonyl compounds (Chumbao *et al.*, 2003; Abele & Lukevics 2000; Itsuna *et al.*, 1990; Abele *et al.*, 2000; Arıcı *et al.*, 2004*a*,*b*).

The benzofuran ring system of the title compound, (I), is planar, with a maximum deviation from the plane of 0.0042 (25) Å for C15 (Fig. 1). In the benzofuran system, all bond lengths agree with values reported in the literature (Allen, 2002). The dihedral angle between the benzofuran ring system and chlorobenzoyl group is 61.50 (4)°. The C1—Cl1 bond distance is close to the values reported in the literature (Allen, 2002).



(I)

Weak intermolecular C—H···O hydrogen-bonding interactions stabilize the crystal packing (Table 1 and Fig. 2).

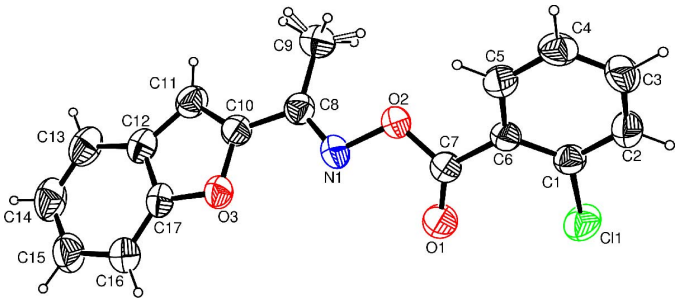


Figure 1
The molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. Both components of the disordered methyl group are shown.

Experimental

For the synthesis of (I), 2-acetylbenzofuranoxime (1.75 g, 10 mmol), triethylamine (2 ml) and dry THF (100 ml) were stirred at room temperature for 1 h. To this solution, 2-chlorobenzoylchloride (1.75 g, 10 mmol) was added dropwise and the mixture was stirred for another 1 h at room temperature. The reaction mixture was poured into water (250 ml) and precipitated twice from water. The solid was filtered off and recrystallized from acetone. Yield 2.92 g, 93.3%.

Crystal data

$C_{17}H_{12}ClNO_3$
M_r = 313.73
Monoclinic, $P2_1/n$
a = 11.9515 (9) Å
b = 8.1082 (4) Å
c = 15.1665 (10) Å
β = 95.359 (6)°
V = 1463.29 (16) Å^3
Z = 4
D_x = 1.424 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 19 482 reflections
θ = 1.7–27.9°
μ = 0.27 mm^{-1}
T = 293 (2) K
Prism, colourless
0.55 × 0.32 × 0.28 mm

Data collection

Stoe IPDS-II diffractometer
φ scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.883, T_{max} = 0.951
19 932 measured reflections
2869 independent reflections
2200 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 26.0°
$h = -14 \rightarrow 14$
$k = -10 \rightarrow 9$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.078
S = 1.02
2869 reflections
199 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0375P)^2 + 0.1959P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}
Extinction correction: none

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O1^{ii}	0.93	2.50	3.213 (2)	134
C16—H16···O1^{i}	0.93	2.55	3.427 (2)	159

Symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, y-1, z$.

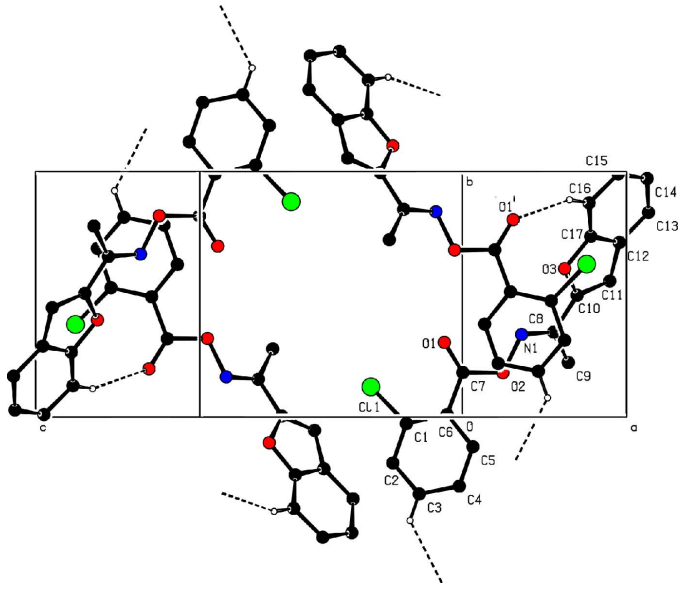


Figure 2
A packing diagram for (I), showing the C—H···O hydrogen bonding interactions as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (i) $\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z$.]

All H atoms were located in difference maps and subsequently treated as riding atoms, with C—H = 0.93 Å (aromatic) and 0.96 Å (CH_3), and with U_{iso}(H) = 1.2U_{eq}($C_{aromatic}$) and 1.5U_{eq}(C_{CH_3}). The methyl group is disordered over two positions with equal occupancy.

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: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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