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(*Z*)-6-Methoxy-4-(2-methoxyimino-2-phenylethoxy)-7-methylisobenzofuran-3(1*H*)-one

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.144
Data-to-parameter ratio = 13.3

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

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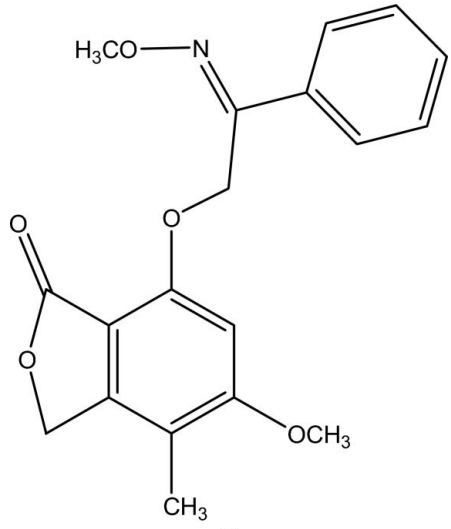
The title compound, $C_{19}H_{19}NO_5$, was synthesized by the reaction of 6-methoxy-4-(2-oxo-2-phenylethoxy)-7-methylisobenzofuran-3(1*H*)-one with *o*-methylhydroxylamine hydrochloride in ethanol. It is a new kind of methoxyimino compound containing isobenzofuran. The dihedral angle between the two six-membered aromatic rings is 104.3 (2)°.

Comment

Much attention has been paid to methyloximes containing diaryl groups (Wang *et al.*, 2005). In view of this, we have recently focused on the preparation of methyloximes that contain isobenzofuran. The title compound, (I), was prepared and its structure determined (Fig. 1).



(I)

The dihedral angle between the two six-membered aromatic rings is 104.3 (2)°. The dihedral angle between the five-membered ring and the fused benzene ring is 0.7°.

Experimental

The title compound was prepared according to the procedure of Wang *et al.* (2005). To a solution of 1,3-dihydro-6-methoxy-4-(2-oxo-2-phenylethoxy)-7-methyl-3-oxo-isobenzofuran (0.312 g, 1 mmol) in EtOH (20 ml) was added a solution of *o*-methylhydroxylamine hydrochloride (0.17 g, 2 mmol) in EtOH (2 ml). The mixture was heated at reflux for 4 h (TLC monitoring) and evaporated to yield a residual solid. This white solid thus obtained was collected and purified by FC (silica gel, 40/60 ethyl acetate–petroleum ether) to give (I) (0.294 g, 86.2%). Colourless single crystals of (I) were grown by slow evaporation of a chloroform–heptane (3:2) solution.

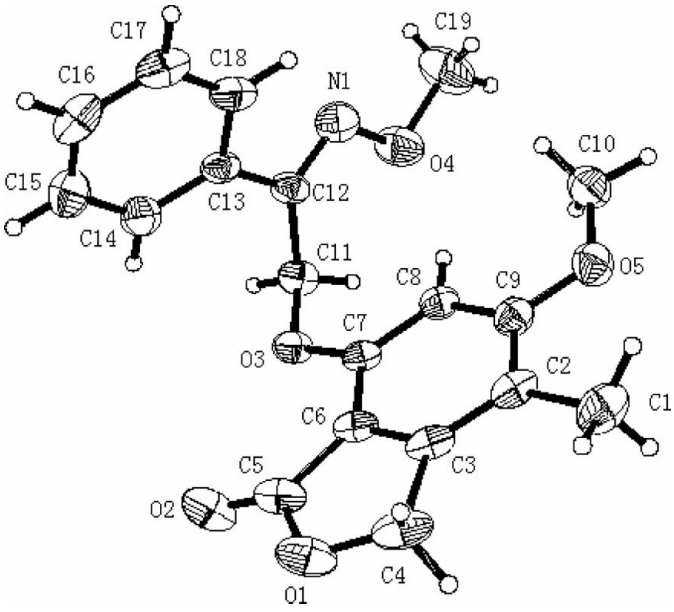


Figure 1
The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids. H atoms are drawn as spheres of arbitrary radius.

Crystal data

$C_{19}H_{19}NO_5$
M_r = 341.35
Monoclinic, $P2_1/c$
a = 9.3964 (2) Å
b = 19.445 (4) Å
c = 9.8521 (2) Å
β = 105.307 (3)°
V = 1736.3 (5) Å^3
Z = 4
D_x = 1.306 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 294 (2) K
Block, colourless
0.30 × 0.26 × 0.20 mm

Data collection

Bruker SMART 1000 diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1990)
T_{min} = 0.972, T_{max} = 0.981
8700 measured reflections
3057 independent reflections
1900 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.144
S = 1.02
3057 reflections
229 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0775P)^2 + 0.1213P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.97 Å), with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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