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7-Methoxy-4,6-dimethyl-3*H*-isobenzofuran-1-one

Jian-Feng Wang,[a] Xin Lin,[a] Yao-Jian Huang,[a] Wen-Jin Su,[a] Yu-Fen Zhao[b] and Seik Weng Ng[c]*

[a]Department of Biology, Xiamen University, Xiamen 361005, People's Republic of China, [b]Department of Chemistry, Xiamen University, Xiamen 361005, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.060
wR factor = 0.156
Data-to-parameter ratio = 7.0

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

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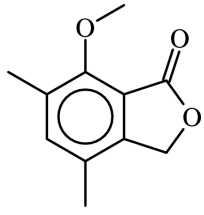
The title compound, $C_{11}H_{12}O_3$, exists as a nearly planar molecule, the dihedral angle between the five- and six-membered rings being 1.9 (2)°.

Comment

7-Methoxy-4,6-dimethyl-3*H*-isobenzofuran-1-one, (I), exists as a nearly planar molecule, the dihedral angle between the five- and six-membered rings being 1.9 (2)°. The compound exhibits moderate cytotoxicity towards the KB cell line (IC_{50} 50 μg ml^{-1}).



(I)

Experimental

The title compound was crystallized from the ethyl acetate extract of the liquid culture of an unidentified marine fungus isolated from the leaves of the sea lotus found in Fujian Province, China.

Crystal data

$C_{11}H_{12}O_3$
M_r = 192.21
Orthorhombic, $Pna2_1$
a = 7.5508 (7) Å
b = 12.616 (1) Å
c = 10.1223 (9) Å
V = 964.27 (15) Å^3
Z = 4
D_x = 1.324 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1595 reflections
θ = 2.6–21.8°
μ = 0.10 mm^{-1}
T = 298 (2) K
Needle, colorless
0.45 × 0.12 × 0.09 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: none
12924 measured reflections
897 independent reflections
840 reflections with $I > 2\sigma(I)$
R_{int} = 0.070
θ_{max} = 25.0°
$h = -8 \rightarrow 8$
$k = -15 \rightarrow 14$
$l = -11 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.156
S = 1.13
897 reflections
129 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.1111P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.342 (6)	C3—C4	1.400 (7)
O1—C2	1.434 (7)	C4—C5	1.381 (7)
O2—C1	1.205 (6)	C4—C9	1.489 (7)
O3—C7	1.361 (6)	C5—C6	1.385 (6)
O3—C11	1.418 (7)	C6—C7	1.381 (6)
C1—C8	1.462 (6)	C6—C10	1.515 (6)
C2—C3	1.480 (7)	C7—C8	1.409 (6)
C3—C8	1.377 (7)		
C1—O1—C2	110.3 (4)	C3—C4—C9	121.1 (4)
C7—O3—C11	117.7 (3)	C4—C5—C6	123.7 (4)
O2—C1—O1	120.4 (5)	C7—C6—C5	120.3 (4)
O2—C1—C8	130.7 (5)	C7—C6—C10	119.3 (4)
O1—C1—C8	108.8 (4)	C5—C6—C10	120.4 (4)
O1—C2—C3	105.2 (4)	O3—C7—C6	118.8 (4)
C8—C3—C4	122.4 (4)	O3—C7—C8	123.5 (4)
C8—C3—C2	108.0 (4)	C6—C7—C8	117.5 (4)
C4—C3—C2	129.6 (5)	C3—C8—C7	120.7 (4)
C5—C4—C3	115.3 (4)	C3—C8—C1	107.7 (4)
C5—C4—C9	123.6 (5)	C7—C8—C1	131.5 (4)

The H atoms were positioned geometrically and were included in the refinement in the riding-model approximation. C—H distances were set to 0.93–0.97 Å, with U_{iso} values for H atoms of 1.2 or 1.5 (methyl H) times U_{eq} of the parent atom. The methyl groups bonded to the aromatic ring were allowed to rotate but not to tip. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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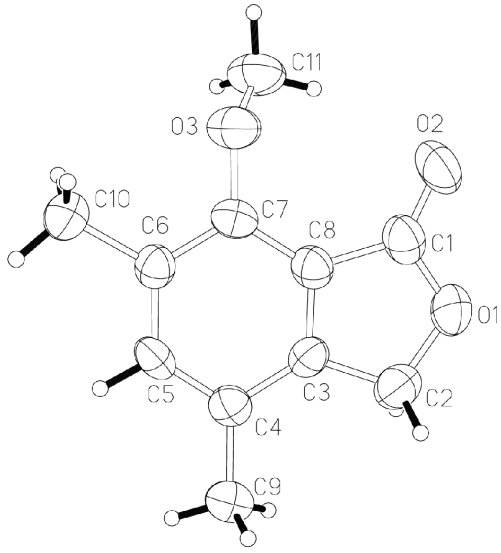

Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

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