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Key indicators
Single-crystal X-ray study
T = 295 K
Mean e(C–C) = 0.003 Å
R factor = 0.053
wR factor = 0.119
Data-to-parameter ratio = 15.3

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, (I), a benzophenone derivative, is an intermediate for the preparation of antimitotic β-apopicropodophyllin (Basavaraju & Anjanamurthy, 2003). Over 300 crystal structures of benzophenone derivatives in the Cambridge Structural Database (CSD, Version 5.26; Allen, 2002) highlight the importance of structural studies on such pharmaceutically useful compounds. The synthesis and structure of (I) are reported here.

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molecule as a whole is essentially described by the torsion angles about the C1—C7 and C7—C8 bonds: C2—C1—C7—
O1 = −7.0 (3), O1—C7—C8—C13 = −50.7 (3), C2—C1—
C7—C8 = 173.61 (16)° and C1—C7—C8—C13 = 128.68 (19)°.
In contrast, the values of the corresponding torsion angles in
an isomeric compound crystallizing in P2₁/c (2-methoxy-5-
methylphenyl phenyl ketone; Malathy Sony et al., 2005) are:
C6—C1—C7—C8 = 51.7 (3), O8—C7—C9—C10 = 17.5 (4),
C6—C1—C7—C9 = −124.9 (3)° and C1—C7—C9—C10
= −166.0 (2)°.

A view of the crystal packing is shown in Fig. 2. The crystal
structure displays a significant short intermolecular
π–π contact of face-to-face type, where the Cg1· · ·Cg1† [symmetry
code: (i) −x, 2 − y, 1 − z; Cg1 is the centroid of the ring C1–
C6] separation and perpendicular distances are 3.55 and 3.48Å,
respectively. The rest of the short intermolecular contacts are in the range of van der Waals interactions.

Experimental
A solution of o-methylanisole (2 g, 0.0163 mol) in dry dichloro-
methane (15 ml) was treated with anhydrous aluminium chloride
(2.183 g, 0.0163 mol). The reaction mixture was stirred continuously
for 30 min. A solution of benzoyl chloride (2.3 g, 0.01637 mol) in
dichloromethane (15 ml) was added dropwise over a period of 1 h to
the reaction mixture at 298 K. After 24 h, 6 ml of concentrated HCl
was added over 30 min. The reaction mixture was stirred for 24 h.
Aqueous NaCl solution (10%) was added over 30 min. The reaction mixture at 298 K. After 24 h, 6 ml of concentrated HCl
dichloromethane (15 ml) was treated with anhydrous aluminium chloride

Table 1
Selected geometric parameters (Å, °).

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<tr>
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<tr>
<td>O1—C7</td>
<td>1.222 (2)</td>
<td>C1—C7</td>
<td>1.480 (3)</td>
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<tr>
<td>O2—C4</td>
<td>1.361 (2)</td>
<td>C3—C14</td>
<td>1.503 (3)</td>
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<tr>
<td>O2—C15</td>
<td>1.425 (2)</td>
<td>C7—C8</td>
<td>1.499 (3)</td>
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<tr>
<td>C4—O2—C15</td>
<td>119.04 (16)</td>
<td>O2—C4—C3</td>
<td>121.16 (18)</td>
</tr>
<tr>
<td>C6—C1—C7</td>
<td>122.93 (16)</td>
<td>C1—C7—C8</td>
<td>119.93 (16)</td>
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<tr>
<td>C2—C1—C7</td>
<td>119.31 (16)</td>
<td>C1—C7—C9</td>
<td>119.16 (18)</td>
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<td>C2—C3—C14</td>
<td>121.87 (17)</td>
<td>C9—C8—C7</td>
<td>124.02 (17)</td>
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<tr>
<td>C4—C3—C14</td>
<td>120.42 (17)</td>
<td>C9—C8—C13</td>
<td>124.25 (17)</td>
</tr>
<tr>
<td>O2—C4—C3</td>
<td>124.29 (17)</td>
<td>C13—C8—C7</td>
<td>120.18 (17)</td>
</tr>
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All H atoms were positioned geometrically and were refined as
riding on their carrier atoms, with Cm—H = 0.93Å with Uiso(H) = 1.2Ueq(Cm), and Cmethyl—H = 0.96Å with Uiso(H) = 1.5Ueq(Cmethyl).

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-
Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to
to solve structure: SHELXTL (Bruker, 2000); program(s) used to refine
structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3
(Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97 and PLATON.

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References
880.
Wisconsin, USA.
Bruker (2001). SMART (Version 5.244) and SAINT-Plus (Version 6.02a).
Bruker AXS Inc., Madison, Wisconsin, USA.
Khanum, S. A., Mahendra, M., Shashikanth, S., Doreswamy, B. H., Sridhar, M. A.
Mahendra, M., Khanum, S. A., Singh, A. K., Shashikanth, S., Doreswamy, B. H.,