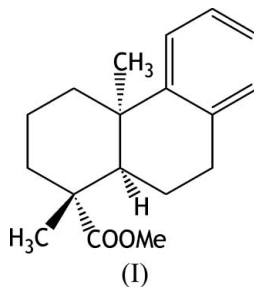


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whengshan@yahoo.com**Key indicators**Single-crystal X-ray study  
 $T = 153\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$   
 $R$  factor = 0.027  
 $wR$  factor = 0.072  
Data-to-parameter ratio = 7.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**Methyl *cis*-deisopropyldehydroabietate**

In the title compound,  $\text{C}_{18}\text{H}_{24}\text{O}_2$ , a derivative of dehydroabietic acid formed by a Friedel–Crafts reaction between methyl dehydroabietate and aluminium trichloride, the fused cyclohexane rings exhibit classical chair and half-chair conformations.

**Comment**

Pine resin is a very abundant renewable source composed mainly of diterpene resin acids of the general formula  $\text{C}_{19}\text{H}_{29}\text{COOH}$ . This raw material has a wide range of industrial uses and is also a source of fine chemicals (Zinkel & Russell, 1989). Dehydroabietic acid derivatives have shown a broad spectrum of biological activities such as antifungal and tumour-inhibitory properties (Silvestre *et al.*, 1998; Fonseca *et al.*, 2004). Considerable interest has been devoted to this easily available compound as a starting material, as either the free acid or the ester, for the synthesis of other important natural or bioactive compounds, mainly through transformations that involve the benzylic or aromatic portions of the molecule (Roy *et al.*, 2003).

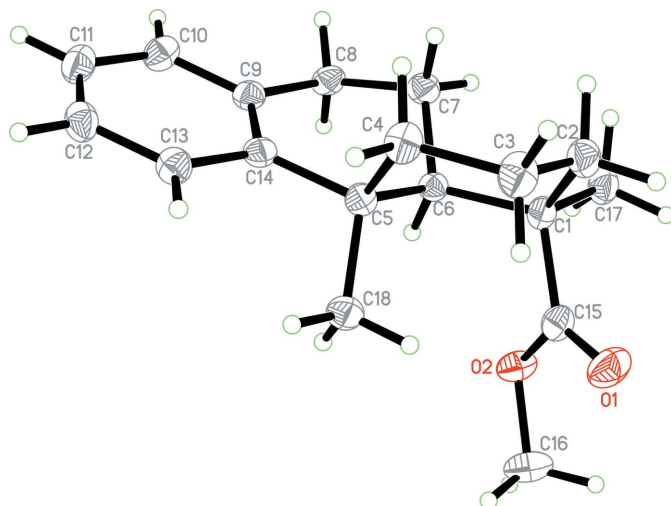


The title compound, (I), is analogous to methyl 12-bromo-13,14-dinitrodeisopropyldehydroabietate (Pan *et al.*, 2005), but without the substituents on the benzene ring (Fig. 1). The fused rings *A* (atoms C1–C6) and *B* (C5–C9/C14) adopt chair and half-chair conformations, respectively. Both the ester at C1 and the methyl group at C5 occupy the axial positions on the cyclohexyl ring. The bond lengths and angles in the molecule are comparable to those in methyl 12-bromo-13,14-dinitrodeisopropyldehydroabietate (Pan *et al.*, 2005) and are in normal ranges (Allen *et al.*, 1987).

The result confirms that during Friedel–Crafts reaction of methyl dehydroabietate, there is cleavage of ring *B* and formation of the intermediate carbenium ion. The carbenium ion has two steric modes of interaction with the benzene ring, so it is not surprising that bond formation occurs on the other side of ring *A*, thus creating the *cis*-product (Baleizão *et al.*, 2004). The packing pattern of molecules is the same as in methyl-12-benzoyl-dehydroabietate (Li *et al.*, 2006).

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**Figure 1**  
The structure of (I), showing 50% probability displacement ellipsoids and the atom-labelling scheme. H atoms are represented by small spheres of arbitrary radius.

## Experimental

Aluminium trichloride (100.4 mmol) was added carefully to a solution of methyl dehydroabietate (17.1 mmol) in toluene (71.7 ml) with vigorous stirring under nitrogen at room temperature for 24 h. The resulting mixture was poured into ice–water. The separated organic layer was then washed with water and dried with anhydrous magnesium sulfate. The aqueous layer was extracted with dimethyl ether, washed with water and dried with anhydrous magnesium sulfate. The organic layers were evaporated to dryness. The residue obtained was dissolved in light petroleum, treated with charcoal and filtered after 24 h. The solution was dried and evaporated leaving a yellow gum. Compound (I) was obtained as colourless crystals (yield 1.63 g, 35%, m.p. 363.4–364.3 K) by recrystallization from absolute methanol.

### Crystal data

$C_{18}H_{24}O_2$   
 $M_r = 272.37$   
Monoclinic,  $P2_1$   
 $a = 8.459$  (2) Å  
 $b = 7.4681$  (19) Å  
 $c = 11.701$  (3) Å  
 $\beta = 95.173$  (5)°  
 $V = 736.1$  (3) Å<sup>3</sup>

$Z = 2$   
 $D_x = 1.229$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 153$  (2) K  
Block, colourless  
0.50 × 0.44 × 0.30 mm

### Data collection

Rigaku Mercury diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan  
(Jacobson, 1998)  
 $T_{\min} = 0.784$ ,  $T_{\max} = 0.978$

7106 measured reflections  
1451 independent reflections  
1436 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.019$   
 $\theta_{\text{max}} = 25.3^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.027$   
 $wR(F^2) = 0.072$   
 $S = 1.05$   
1451 reflections  
185 parameters  
H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0435P)^2 + 0.1277P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$

H atoms bound to C atoms were positioned geometrically and included in the refinement in the riding-model approximation (C–H = 0.95, 0.98, 0.99 and 1.00 Å for aromatic, methyl, CH<sub>2</sub> and CH groups, respectively) and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms and  $1.2U_{\text{eq}}(\text{C})$  for all others.

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSK, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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