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whengshan@yahoo.com**Key indicators**

Single-crystal X-ray study

T = 193 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.036

wR factor = 0.086

Data-to-parameter ratio = 7.6

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Maleopimaric acid trimethyl ester**

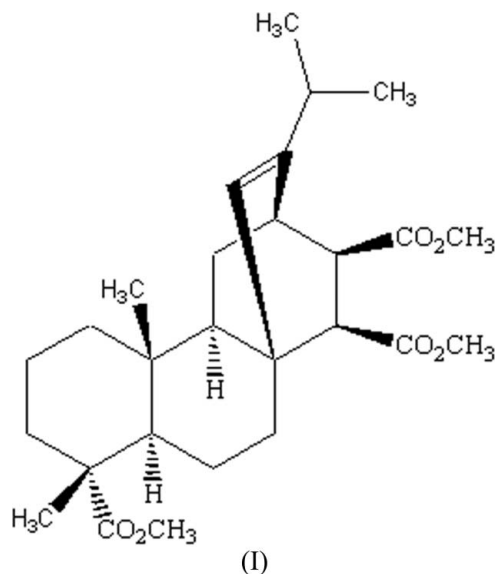
The title compound, $\text{C}_{27}\text{H}_{40}\text{O}_6$, contains two fused cyclohexane rings with chair conformations, fused to a norbornene ring system. The ester groups that are attached to the norbornene unit are in a *cis* configuration. There are two molecules in the asymmetric unit. The structure is stabilized by $\text{C}-\text{H} \cdots \text{O}$ intermolecular hydrogen bonds and van der Waals forces.

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Comment

Maleopimaric acid (Zalkov *et al.*, 1962) is a derivative of abietic acid, an important resin acid (Lee *et al.*, 2001) used in materials processing, such as in surface active agents and paints. It is also a useful intermediate for natural product synthesis (Khlebnikova *et al.*, 2004).



The title compound, (I), is an ester derivative of maleopimaric acid (Fig. 1). The asymmetric unit consists of two independent molecules. Each molecule contains two fused cyclohexane rings with chair conformations and a fused norbornene ring system. The C1–C6 and C28–C33 six-membered rings display boat conformations. The H atoms on atoms C1, C2, C5 and C11 in the first molecule and C28, C29, C32 and C38 in the second molecule occupy axial positions, which are similar to those in a derivative of abietic acid (Li *et al.*, 2005). The ester groups at C1/C2 and C28/C29 are in *cis* positions as expected (Zalkov *et al.*, 1962). The configuration about the C7=C8 and C34=C35 bonds in the two molecules is *Z*, where the H atom and the isopropyl group are *cis*. All the bond lengths and angles are in normal ranges (Allen *et al.*,

1987). In the crystal structure, the molecules are linked (Fig. 2) by C—H...O intermolecular hydrogen bonds (Table 2) and van der Waals forces.

Experimental

Maleopimaric acid was prepared according to a literature procedure (Zalkov *et al.*, 1962). To a 50 ml three-necked flask were added maleopimaric acid (4.0 g, 4 mmol) and phosphorus trichloride (3 ml, 34.3 mol). The mixture was stirred vigorously with a magnetic stirrer at room temperature for 4 h. After removing the solvent under vacuum, anhydrous methanol (20 ml) was added to the residue and refluxed for 3 h. The mixture was cooled to room temperature and then filtered. The colorless solid formed was recrystallized from ethanol (2.9 g, yield 63%, m.p. 375–377 K).

Crystal data

C₂₇H₄₀O₆ Z = 4
M_r = 460.59 *D_x* = 1.240 Mg m⁻³
 Monoclinic, *P*2₁ Mo *K*α radiation
a = 8.9848 (15) Å μ = 0.09 mm⁻¹
b = 23.456 (4) Å *T* = 193 (2) K
c = 12.364 (2) Å Plate, colorless
 β = 108.804 (3)° 0.79 × 0.60 × 0.12 mm
V = 2466.6 (7) Å³

Data collection

Rigaku Mercury diffractometer 24150 measured reflections
 ω scans 4615 independent reflections
 Absorption correction: multi-scan 4475 reflections with *I* > 2σ(*I*)
 (Jacobson, 1998) *R*_{int} = 0.026
*T*_{min} = 0.804, *T*_{max} = 0.990 θ_{max} = 25.3°

Refinement

Refinement on *F*² *w* = 1/[σ²(*F*_o²) + (0.0442*P*)²
R[*F*² > 2σ(*F*²)] = 0.036 + 0.5815*P*]
wR(*F*²) = 0.086 where *P* = (*F*_o² + 2*F*_c²)/3
S = 1.07 (Δ/σ)_{max} < 0.001
 4615 reflections Δρ_{max} = 0.41 e Å⁻³
 610 parameters Δρ_{min} = -0.16 e Å⁻³
 H-atom parameters constrained

Table 1

Selected bond lengths (Å).

O1—C17	1.205 (3)	O5—C25	1.201 (3)
O2—C17	1.348 (3)	O6—C25	1.342 (3)
O3—C19	1.203 (4)	C7—C8	1.330 (3)
O4—C19	1.344 (3)		

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C2—H2...O11 ⁱ	1.00	2.47	3.357 (3)	147
C18—H18C...O3 ⁱⁱⁱ	0.98	2.56	3.377 (4)	141
C26—H26C...O1 ⁱⁱⁱ	0.98	2.51	3.389 (4)	149
C29—H29...O5	1.00	2.49	3.386 (3)	150
C53—H53C...O9 ^{iv}	0.98	2.60	3.513 (4)	156

Symmetry codes: (i) *x* - 1, *y*, *z*; (ii) *x* + 1, *y*, *z*; (iii) -*x* + 1, *y* + ½, -*z* + 1; (iv) -*x* + 2, *y* - ½, -*z* + 2.

H atoms were positioned geometrically and included in the refinement in the riding-model approximation, with C—H = 0.95, 0.98, 0.99 and 1.00 Å for aromatic, methyl, CH₂ and CH groups,

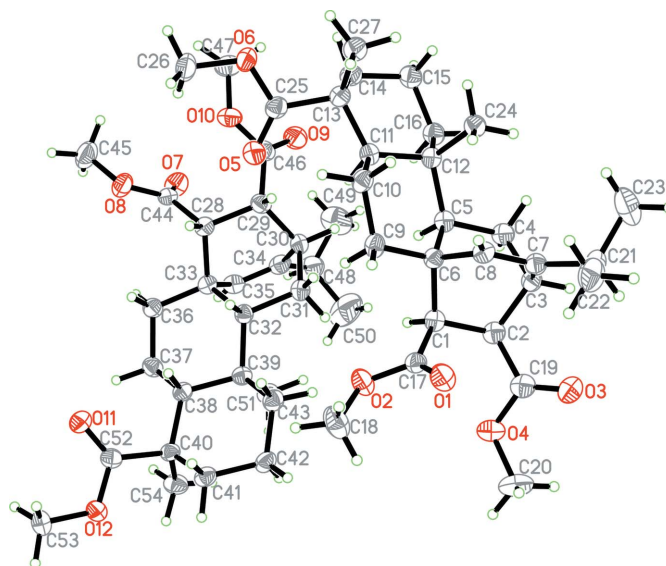


Figure 1

The structures of the two independent molecules in the asymmetric unit of (I), showing the atom-labeling scheme and 50% probability displacement ellipsoids. H atoms are represented by small spheres of arbitrary radii.

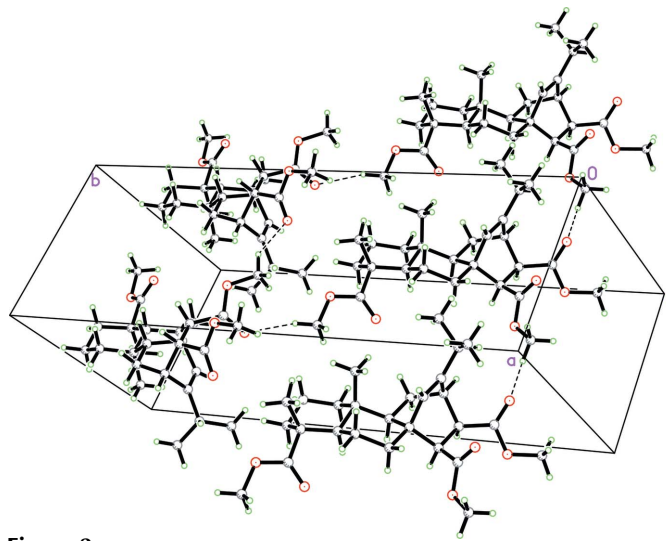


Figure 2

Packing diagram for (I). Hydrogen bonds are denoted by dashed lines.

respectively, and with *U*_{iso}(H) = 1.5*U*_{eq}(methyl C) and 1.2*U*_{eq}(other C). In the absence of significant anomalous scattering effects, Friedel pairs were merged.

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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