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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.046
 wR factor = 0.115
Data-to-parameter ratio = 14.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.2-Methyl-6-(1,7,7-trimethylbicyclo[2.2.1]-
hept-2-yl)phenol

In the title compound, $\text{C}_{17}\text{H}_{24}\text{O}$, the six-membered ring of the bicyclo[2.2.1]heptyl moiety has a boat conformation and the phenol group is in an equatorial position. In the crystal structure, centrosymmetric dimers are formed *via* intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds with rather unfavorable geometry.

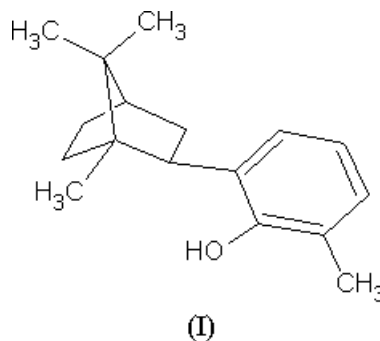
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Comment

The title compound, (I), belongs to the class of terpeno-phenolic compounds. Some of these compounds are natural products and possess biological activity (Banthorpe & Charlwood, 1972). Others, like (I), are widely used as antioxidants in industry and as starting components in the synthesis of some drugs and fragrant substances (Kuzakov & Shmidt, 2000; Swift, 2004) or in asymmetric syntheses (Berkessel *et al.*, 2002). Thus, the synthesis and structure of (I) and similar compounds is of great importance (Chukicheva *et al.*, 2003).



The present crystallographic study has shown that all bond lengths and angles in (I) are close to standard values. The C1–C6 six-membered ring has a boat conformation (Fig. 1). Atoms C1 and C4 deviate from the plane of the remaining atoms of the ring by 0.909 (3) and 0.809 (3) Å, respectively. The methyl group at C1 and the phenol group at C2 are in equatorial positions (Table 1).

In the crystal structure, molecules form centrosymmetric dimers *via* $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2). However, this hydrogen bond possesses rather unfavorable geometry ($\text{O}-\text{H}\cdots\text{O} = 118^\circ$), probably because of the presence of the substituents in both *ortho* positions of the phenol ring and sterically restricts an incoming acceptor of the hydrogen bond. It is also of note that the distance (2.19 Å) between H atoms ($\text{H1}\cdots\text{H1}^i$) (symmetry code as in Table 2) in the dimer is considerably shorter than the sum of the van der Waals radii for two H atoms (2.32 Å; Zefirov & Zorky, 1989).

Experimental

The synthesis of (I) was recently reported (Chukicheva *et al.*, 2003). The crystals were grown by isothermal evaporation of a solution of (I) in hexane.

Crystal data

$C_{17}H_{24}O$	$Z = 2$
$M_r = 244.36$	$D_x = 1.139 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 7.252(4) \text{ \AA}$	Cell parameters from 24 reflections
$b = 7.442(4) \text{ \AA}$	$\theta = 10\text{--}11^\circ$
$c = 13.430(8) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$\alpha = 93.49(5)^\circ$	$T = 293(2) \text{ K}$
$\beta = 98.74(5)^\circ$	Prism, colorless
$\gamma = 94.56(5)^\circ$	$0.50 \times 0.20 \times 0.20 \text{ mm}$
$V = 712.2(7) \text{ \AA}^3$	

Data collection

Siemens P3 diffractometer	$\theta_{\text{max}} = 25.1^\circ$
$\theta/2\theta$ scans	$h = 0 \rightarrow 8$
Absorption correction: none	$k = -8 \rightarrow 8$
2682 measured reflections	$l = -15 \rightarrow 15$
2468 independent reflections	2 standard reflections
1213 reflections with $I > 2\sigma(I)$	every 98 reflections
$R_{\text{int}} = 0.046$	intensity decay: 3.2%

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.046$	$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2]$
$wR(F^2) = 0.115$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.79$	$(\Delta/\sigma)_{\text{max}} = 0.001$
2468 reflections	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
167 parameters	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$

Table 1

Selected torsion angles ($^\circ$).

C6—C1—C2—C12	−149.02 (17)	C5—C4—C7—C9	173.10 (19)
C8—C1—C6—C5	163.92 (18)	C6—C1—C7—C10	60.1 (2)
C3—C4—C7—C9	60.5 (2)	C2—C1—C7—C10	167.18 (16)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O1—H1 \cdots O1 ⁱ	0.82	2.45	2.933 (3)	118

Symmetry code: (i) $-x, 2 - y, -z$.

All H atoms were located in difference Fourier syntheses. All methyl H atoms were refined as part of a rigid group, which was allowed to rotate but not tip or distort, and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$. Other H atoms were refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The bond distances were

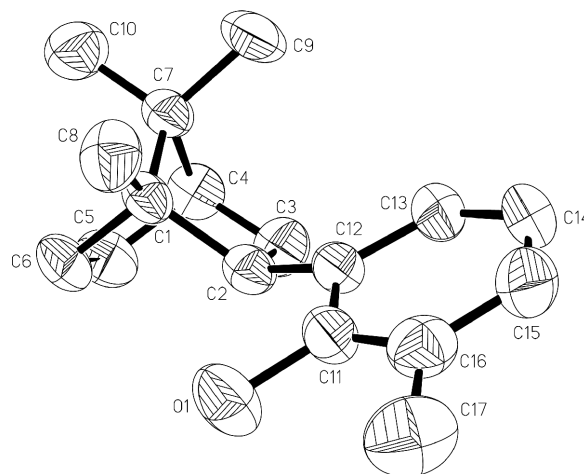


Figure 1

The molecular structure of (I), showing displacement ellipsoids at the 50% probability level. H atoms have been omitted.

constrained: methyl C—H = 0.96 \AA , methylene C—H = 0.97 \AA , methine C—H = 0.98 \AA , aromatic C—H = 0.93 \AA and O—H = 0.82 \AA .

Data collection: *P3 Diffractometer Control Program* (Siemens, 1989); cell refinement: *P3 Diffractometer Control Program*; data reduction: *XDISK* (Siemens, 1991); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXL97*.

P3 and *XDISK* software packages were accessed via the X-ray Structural Centre, Moscow. The author thanks Dr A. V. Kuchin for help in obtaining crystals of (I).

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