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2-Methyl-4-phenylbuta-2,3-dien-1-ol

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.011 Å
R factor = 0.039
wR factor = 0.084
Data-to-parameter ratio = 8.3

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

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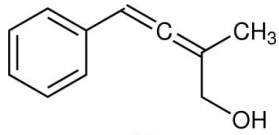
The crystal structure of the title compound, $C_{11}H_{12}O$, a substrate for gold-catalysed cycloisomerization reactions [Hoffmann-Röder & Krause (2001). *Org. Lett.* **3**, 2537–2538], contains two molecules in the asymmetric unit. There are two intermolecular O—H ··· O hydrogen bonds in the crystal structure and a chain of molecules is formed along the *c* axis *via* these hydrogen bonds.



(I)

Experimental

The title compound was synthesized in racemic form by S_N2'-substitution of a propargyl oxirane with a magnesium cuprate (Krause & Hoffmann-Röder, 2004). It was dissolved in a small amount of ethyl acetate/cyclohexane (1:4 *v*/*v*), and crystals were obtained by slow evaporation of the mixed solution.

Crystal data

$C_{11}H_{12}O$
M_r = 160.21
Orthorhombic, $Pca2_1$
a = 24.379 (6) Å
b = 9.601 (2) Å
c = 7.991 (3) Å
V = 1870.4 (9) Å^3
Z = 8
D_x = 1.138 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 17261 reflections
θ = 3.1–25.1°
μ = 0.07 mm^{-1}
T = 173 (1) K
Needle, colourless
0.15 × 0.08 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
ω scans
Absorption correction: none
17261 measured reflections
1832 independent reflections
578 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 25.5°
$h = -29 \rightarrow 29$
$k = -11 \rightarrow 11$
$l = -9 \rightarrow 9$

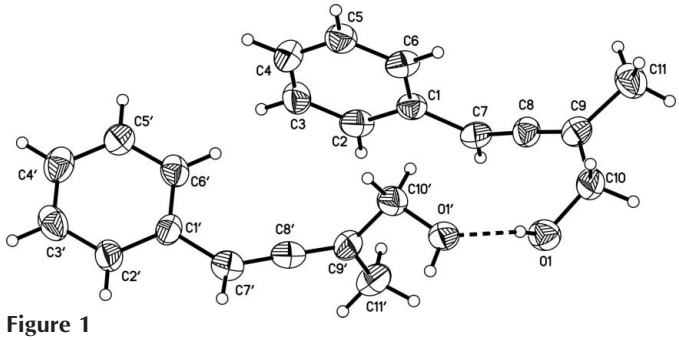


Figure 1
The asymmetric unit of the title compound, showing the labelling of all non-H atoms. The dashed line indicates an intermolecular hydrogen bond. Displacement ellipsoids are drawn at the 30% probability level.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.084$
$S = 1.00$
1832 reflections
221 parameters
H-atom parameters constrained
$w = [\exp(4.2(\sin\theta/\lambda)^2)]/[\sigma^2(F_o^2)]$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.11$ e Å^{-3}
$\Delta\rho_{min} = -0.11$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1′	0.84	1.91	2.717 (6)	162
O1′—H1′···O1^{i}	0.84	1.95	2.739 (6)	157

Symmetry code: (i) $-x, -y-1, z+\frac{1}{2}$.

In the absence of significant anomalous dispersion effects, Friedel pairs were merged. H atoms were placed in calculated positions, with C—H = 0.95–0.99 Å and O—H = 0.84 Å, and were refined as riding, with U_{iso}(H) = 1.5U_{eq}(C,O) for methyl and hydroxyl groups and 1.2U_{eq}(C) for others; the methyl and the hydroxyl groups were allowed to rotate but not to tip.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*, *PARST95* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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