4-(4-Ethylcyclohexyl)phenol

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.044
wR factor = 0.127
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.

The crystal structure of the title compound, $C_{14}H_{20}O$, is stabilized by a disordered O—H···O hydrogen bond.

Comment

Phenol derivatives are widely used as starting materials for many products, including drugs and liquid crystalline materials (Eidenschink *et al.*, 1978). The title compound, (I) (Fig. 1), has been synthesized from 4-(4-ethylcyclohexyl)acetophenone. The bond lengths and angles are within their normal ranges. The cyclohexyl ring adopts a chair conformation and the structure is stabilized by O—H···O hydrogen bonds (Table 1). The H atom of the hydroxy group was found to be disordered over two sites, with equal occupancies.

(I)
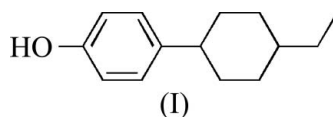
Experimental

The title compound was prepared according to the procedure of Hu *et al.* (2003). Suitable crystals of (I) (m.p. 400–402 K) were obtained by slow evaporation of a methanol solution.

Crystal data

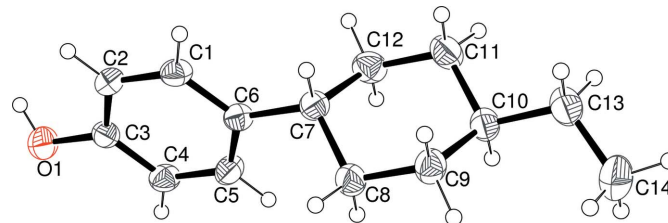|	
$C_{14}H_{20}O$	$Z = 4$
$M_r = 204.30$	$D_x = 1.148$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 16.121$ (5) Å	$\mu = 0.07$ mm^{-1}
$b = 5.4451$ (17) Å	$T = 294$ (2) K
$c = 13.478$ (4) Å	Block, colourless
$\beta = 92.727$ (6)°	$0.24 \times 0.20 \times 0.18$ mm
$V = 1181.7$ (6) Å^3	

Figure 1
The molecular structure of (I), shown with 40% displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. Only one of the disordered H atoms attached to O1 is shown.

Data collection

Bruker SMART CCD
  diffractometer
ω scans
Absorption correction: multi-scan
  (*SADABS*; Sheldrick, 1996)
  $T_{min} = 0.978$, $T_{max} = 0.988$

5722 measured reflections
2101 independent reflections
1198 reflections with $I > 2\sigma(I)$
$R_{int} = 0.040$
$\theta_{max} = 25.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.127$
$S = 1.01$
2101 reflections
137 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0609P)^2$
  $+ 0.0454P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.14$ e Å^{-3}
$\Delta\rho_{min} = -0.14$ e Å^{-3}

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
O1—H1$A\cdots$O1^i	0.84	2.05	2.893 (3)	180
O1—H1$B\cdots$O1^{ii}	0.84	2.11	2.953 (3)	179

Symmetry codes: (i) $-x, -y, -z$; (ii) $-x, -y + 1, -z$.

To avoid an unreasonable intermolecular H$\cdots$H contact, the H atom of the OH group must be disordered over two positions with equal occupancy so as to form alternative O—H$\cdots$O bonds to adjacent OH groups. These atoms were positioned geometrically and refined as riding. All C-bound H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined using a riding model, with $U_{iso}(H)$ = 1.2$U_{eq}(C)$ or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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