organic compounds

4-(4-n-Propylcyclohexyl)phenol

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In the title compound, $C_{15}H_{22}O$, the cyclohexyl ring adopts a chair conformation. The crystal structure is stabilized by a disordered O—H···O hydrogen bond which forms zigzag chains along the b axis.

Related literature

For a related structure, see Wang *et al.* (2006); for uses of phenol derivatives, see Eidenschink *et al.* (1978). For related literature, see Hu *et al.* (2003).
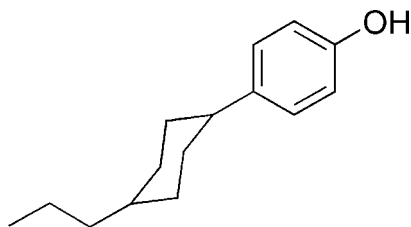
Experimental

Crystal data

$C_{15}H_{22}O$
$M_r = 218.33$
Monoclinic, $C2/c$
$a = 35.062$ (5) Å
$b = 5.3648$ (6) Å
$c = 13.488$ (2) Å
$\beta = 98.994$ (6)°
$V = 2505.9$ (6) Å^3
$Z = 8$
Mo $K\alpha$ radiation
$\mu = 0.07$ mm^{-1}
$T = 113$ (2) K
$0.20 \times 0.14 \times 0.10$ mm

Data collection

Rigaku Saturn CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.986$, $T_{max} = 0.993$
8805 measured reflections
2182 independent reflections
1824 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.130$
$S = 1.13$
2182 reflections
153 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···O1[i]	0.821 (10)	2.060 (14)	2.867 (3)	168 (4)
O1—H1A···O1[ii]	0.817 (10)	2.083 (12)	2.893 (3)	171 (4)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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: *CrystalStructure* (Rigaku/MSC, 2005).

References

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Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, H.-F., Guo, Y., Zhang, H., Zeng, T. & Li, H.-B. (2006). *Acta Cryst.* E**62**, o3721–o3722.

supplementary materials

4-(4-*n*-Propylcyclohexyl)phenol

H.-X. Zhang, B.-H. Tang and X.-H. Jin

Comment

Phenol derivatives are widely used as starting materials for many products, including drugs and liquid crystalline materials (Eidenschink *et al.*, 1978) and the crystal structure of 4-(4-n-propylcyclohexyl)phenol is reported herein, Fig. 1. The cyclohexyl ring adopts a chair conformation and the molecules were linked into dimers by O—H···O hydrogen bonds (Table 1).

Experimental

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

Refinement

To avoid an unreasonable intermolecular H···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···O bonds to adjacent OH groups. The H atoms of the disordered O—H groups were refined freely with fixed isotropic displacement parameters, $U_{iso} = 1.5U_{eq}$ (O). Other H atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, $U_{iso}=1.2U_{eq}$ (C) for aromatic 1.00 Å, $U_{iso} = 1.2U_{eq}$ (C) for CH, 0.99 Å, $U_{iso} = 1.2U_{eq}$ (C) for CH$_2$ and 0.98 Å, $U_{iso} = 1.5U_{eq}$ (C) for CH$_3$ atoms.

Figures
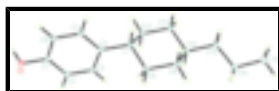
Fig. 1. A view of the molecule of (I), shown with 30% displacement ellipsoids. H atoms are shown as small spheres of arbitrary radii. Only one of the disordered H atoms attached to O1 is shown.

4-(4-n-propylcyclohexyl)phenol

Crystal data

C$_{15}$H$_{22}$O	F_{000} = 960
M_r = 218.33	D_x = 1.157 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71070 Å
Hall symbol: -C 2yc	Cell parameters from 1756 reflections
a = 35.062 (5) Å	θ = 3.1–25.0º
b = 5.3648 (6) Å	μ = 0.07 mm^{-1}
c = 13.488 (2) Å	*T* = 113 (2) K
β = 98.994 (6)º	Prism, colorless
V = 2505.9 (6) Å^3	0.20 × 0.14 × 0.10 mm

$Z = 8$

Data collection

Rigaku Saturn CCD diffractometer	2182 independent reflections
Radiation source: Rotating anode	1824 reflections with $I > 2\sigma(I)$
Monochromator: confocal	$R_{int} = 0.053$
Detector resolution: 7.31 pixels mm^{-1}	$\theta_{max} = 25.0°$
$T = 113(2)$ K	$\theta_{min} = 2.4°$
ω scans	$h = -41 \rightarrow 41$
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)	$k = -6 \rightarrow 6$
$T_{min} = 0.986$, $T_{max} = 0.993$	$l = -15 \rightarrow 16$
8805 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.058$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 1.3717P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.13$	$(\Delta/\sigma)_{max} < 0.001$
2182 reflections	$\Delta\rho_{max} = 0.18$ e Å^{-3}
153 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	y	z	$U_{iso}*/U_{eq}$	Occ. (<1)
O1	0.24200 (4)	0.0013 (2)	0.52977 (10)	0.0218 (4)	

H1A	0.2474 (13)	−0.144 (3)	0.519 (3)	0.033*	0.50
H1B	0.2432 (13)	0.143 (4)	0.508 (3)	0.033*	0.50
C1	0.21933 (5)	0.0111 (3)	0.60602 (13)	0.0159 (4)	
C2	0.19413 (5)	0.2098 (3)	0.60899 (13)	0.0176 (4)	
H2	0.1922	0.3367	0.5593	0.021*	
C3	0.17169 (5)	0.2212 (3)	0.68538 (13)	0.0167 (4)	
H3	0.1546	0.3580	0.6875	0.020*	
C4	0.17364 (5)	0.0360 (3)	0.75906 (13)	0.0162 (4)	
C5	0.19938 (5)	−0.1608 (3)	0.75345 (13)	0.0168 (4)	
H5	0.2013	−0.2891	0.8025	0.020*	
C6	0.22232 (5)	−0.1743 (3)	0.67816 (13)	0.0175 (4)	
H6	0.2398	−0.3090	0.6763	0.021*	
C7	0.14826 (5)	0.0456 (3)	0.84070 (13)	0.0164 (4)	
H7	0.1574	−0.0876	0.8907	0.020*	
C8	0.15084 (5)	0.2951 (4)	0.89706 (14)	0.0192 (4)	
H8A	0.1780	0.3258	0.9274	0.023*	
H8B	0.1428	0.4312	0.8487	0.023*	
C9	0.12539 (5)	0.2995 (4)	0.97970 (13)	0.0183 (4)	
H9A	0.1271	0.4661	1.0116	0.022*	
H9B	0.1352	0.1755	1.0319	0.022*	
C10	0.08291 (5)	0.2411 (3)	0.93881 (14)	0.0171 (4)	
H10	0.0729	0.3761	0.8906	0.021*	
C11	0.08033 (5)	−0.0057 (4)	0.88091 (14)	0.0216 (5)	
H11A	0.0883	−0.1434	0.9285	0.026*	
H11B	0.0531	−0.0351	0.8504	0.026*	
C12	0.10566 (5)	−0.0096 (4)	0.79842 (14)	0.0191 (4)	
H12A	0.0961	0.1165	0.7469	0.023*	
H12B	0.1038	−0.1753	0.7657	0.023*	
C13	0.05754 (5)	0.2345 (4)	1.02191 (14)	0.0202 (5)	
H13A	0.0310	0.1859	0.9916	0.024*	
H13B	0.0676	0.1035	1.0709	0.024*	
C14	0.05541 (6)	0.4796 (4)	1.07852 (15)	0.0245 (5)	
H14A	0.0816	0.5235	1.1129	0.029*	
H14B	0.0468	0.6135	1.0296	0.029*	
C15	0.02804 (6)	0.4687 (4)	1.15591 (15)	0.0279 (5)	
H15A	0.0279	0.6304	1.1897	0.042*	
H15B	0.0367	0.3392	1.2056	0.042*	
H15C	0.0019	0.4294	1.1222	0.042*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0242 (7)	0.0202 (8)	0.0233 (8)	0.0003 (7)	0.0111 (6)	−0.0012 (7)
C1	0.0154 (9)	0.0173 (11)	0.0155 (9)	−0.0038 (7)	0.0040 (7)	−0.0047 (8)
C2	0.0186 (9)	0.0172 (11)	0.0168 (10)	−0.0011 (8)	0.0021 (8)	0.0012 (8)
C3	0.0176 (9)	0.0129 (10)	0.0194 (10)	0.0013 (7)	0.0025 (8)	−0.0019 (8)
C4	0.0156 (9)	0.0167 (11)	0.0157 (9)	−0.0041 (7)	0.0010 (7)	−0.0025 (8)
C5	0.0197 (9)	0.0145 (10)	0.0159 (9)	−0.0009 (8)	0.0014 (8)	0.0011 (8)

C6	0.0164 (9)	0.0142 (10)	0.0219 (10)	0.0018 (7)	0.0032 (8)	−0.0002 (8)
C7	0.0193 (9)	0.0156 (10)	0.0146 (9)	0.0011 (8)	0.0035 (7)	0.0001 (8)
C8	0.0169 (9)	0.0200 (11)	0.0213 (10)	−0.0022 (8)	0.0044 (8)	−0.0030 (8)
C9	0.0168 (9)	0.0213 (11)	0.0169 (10)	−0.0003 (8)	0.0033 (7)	−0.0035 (8)
C10	0.0166 (9)	0.0179 (11)	0.0174 (10)	−0.0003 (8)	0.0043 (8)	0.0004 (8)
C11	0.0195 (9)	0.0232 (12)	0.0229 (10)	−0.0063 (8)	0.0061 (8)	−0.0036 (9)
C12	0.0189 (10)	0.0175 (11)	0.0212 (10)	−0.0029 (8)	0.0038 (8)	−0.0040 (8)
C13	0.0188 (10)	0.0225 (11)	0.0198 (10)	−0.0019 (8)	0.0046 (8)	0.0013 (9)
C14	0.0235 (10)	0.0279 (12)	0.0232 (10)	−0.0017 (9)	0.0074 (8)	−0.0030 (9)
C15	0.0240 (11)	0.0379 (14)	0.0231 (11)	0.0047 (9)	0.0077 (9)	−0.0009 (10)

Geometric parameters (Å, °)

O1—C1	1.396 (2)	C9—C10	1.537 (2)
O1—H1A	0.817 (10)	C9—H9A	0.9900
O1—H1B	0.821 (10)	C9—H9B	0.9900
C1—C6	1.384 (2)	C10—C11	1.533 (2)
C1—C2	1.389 (2)	C10—C13	1.536 (2)
C2—C3	1.392 (2)	C10—H10	1.0000
C2—H2	0.9500	C11—C12	1.528 (2)
C3—C4	1.399 (2)	C11—H11A	0.9900
C3—H3	0.9500	C11—H11B	0.9900
C4—C5	1.399 (2)	C12—H12A	0.9900
C4—C7	1.521 (2)	C12—H12B	0.9900
C5—C6	1.393 (2)	C13—C14	1.528 (3)
C5—H5	0.9500	C13—H13A	0.9900
C6—H6	0.9500	C13—H13B	0.9900
C7—C8	1.535 (2)	C14—C15	1.526 (2)
C7—C12	1.542 (2)	C14—H14A	0.9900
C7—H7	1.0000	C14—H14B	0.9900
C8—C9	1.533 (2)	C15—H15A	0.9800
C8—H8A	0.9900	C15—H15B	0.9800
C8—H8B	0.9900	C15—H15C	0.9800
C1—O1—H1A	110 (3)	H9A—C9—H9B	107.9
C1—O1—H1B	107 (3)	C11—C10—C13	110.92 (15)
H1A—O1—H1B	143 (5)	C11—C10—C9	109.61 (15)
C6—C1—C2	120.65 (16)	C13—C10—C9	112.45 (15)
C6—C1—O1	120.11 (16)	C11—C10—H10	107.9
C2—C1—O1	119.23 (16)	C13—C10—H10	107.9
C1—C2—C3	119.38 (17)	C9—C10—H10	107.9
C1—C2—H2	120.3	C12—C11—C10	112.82 (15)
C3—C2—H2	120.3	C12—C11—H11A	109.0
C2—C3—C4	121.60 (17)	C10—C11—H11A	109.0
C2—C3—H3	119.2	C12—C11—H11B	109.0
C4—C3—H3	119.2	C10—C11—H11B	109.0
C5—C4—C3	117.25 (16)	H11A—C11—H11B	107.8
C5—C4—C7	121.34 (16)	C11—C12—C7	111.58 (15)
C3—C4—C7	121.39 (16)	C11—C12—H12A	109.3
C6—C5—C4	122.00 (17)	C7—C12—H12A	109.3

C6—C5—H5	119.0	C11—C12—H12B	109.3
C4—C5—H5	119.0	C7—C12—H12B	109.3
C1—C6—C5	119.11 (17)	H12A—C12—H12B	108.0
C1—C6—H6	120.4	C14—C13—C10	115.06 (15)
C5—C6—H6	120.4	C14—C13—H13A	108.5
C4—C7—C8	113.09 (15)	C10—C13—H13A	108.5
C4—C7—C12	111.62 (14)	C14—C13—H13B	108.5
C8—C7—C12	109.21 (14)	C10—C13—H13B	108.5
C4—C7—H7	107.6	H13A—C13—H13B	107.5
C8—C7—H7	107.6	C15—C14—C13	113.18 (16)
C12—C7—H7	107.6	C15—C14—H14A	108.9
C9—C8—C7	112.19 (15)	C13—C14—H14A	108.9
C9—C8—H8A	109.2	C15—C14—H14B	108.9
C7—C8—H8A	109.2	C13—C14—H14B	108.9
C9—C8—H8B	109.2	H14A—C14—H14B	107.8
C7—C8—H8B	109.2	C14—C15—H15A	109.5
H8A—C8—H8B	107.9	C14—C15—H15B	109.5
C8—C9—C10	112.17 (15)	H15A—C15—H15B	109.5
C8—C9—H9A	109.2	C14—C15—H15C	109.5
C10—C9—H9A	109.2	H15A—C15—H15C	109.5
C8—C9—H9B	109.2	H15B—C15—H15C	109.5
C10—C9—H9B	109.2		
C6—C1—C2—C3	−0.1 (3)	C4—C7—C8—C9	−179.37 (14)
O1—C1—C2—C3	−179.52 (16)	C12—C7—C8—C9	55.69 (19)
C1—C2—C3—C4	−0.5 (3)	C7—C8—C9—C10	−56.2 (2)
C2—C3—C4—C5	0.6 (3)	C8—C9—C10—C11	53.8 (2)
C2—C3—C4—C7	−178.30 (16)	C8—C9—C10—C13	177.63 (15)
C3—C4—C5—C6	0.0 (3)	C13—C10—C11—C12	−179.05 (15)
C7—C4—C5—C6	178.89 (16)	C9—C10—C11—C12	−54.3 (2)
C2—C1—C6—C5	0.7 (3)	C10—C11—C12—C7	56.5 (2)
O1—C1—C6—C5	−179.91 (16)	C4—C7—C12—C11	178.71 (15)
C4—C5—C6—C1	−0.7 (3)	C8—C7—C12—C11	−55.5 (2)
C5—C4—C7—C8	128.81 (18)	C11—C10—C13—C14	−175.11 (16)
C3—C4—C7—C8	−52.4 (2)	C9—C10—C13—C14	61.8 (2)
C5—C4—C7—C12	−107.56 (19)	C10—C13—C14—C15	176.55 (16)
C3—C4—C7—C12	71.2 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···O1[i]	0.821 (10)	2.060 (14)	2.867 (3)	168 (4)
O1—H1A···O1[ii]	0.817 (10)	2.083 (12)	2.893 (3)	171 (4)

Symmetry codes: (i) −*x*+1/2, −*y*+1/2, −*z*+1; (ii) −*x*+1/2, −*y*−1/2, −*z*+1.

Fig. 1