Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-*tert*-Butyl-4-methyl-6-(4-piperidylmethyl)phenol

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.058
wR factor = 0.155
Data-to-parameter ratio = 16.4

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

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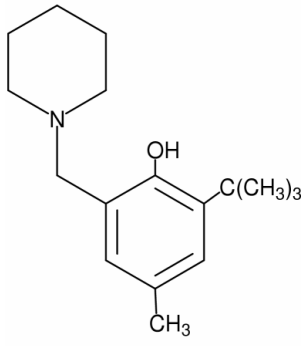
In the title compound, $C_{17}H_{27}NO$, the piperidine ring is folded into the normal chair conformation. There exists an intramolecular O—H···N hydrogen bond involving the N-donor of the piperidine ring.

Received 9 April 2001
Accepted 17 April 2001
Online 10 May 2001

Comment

A great deal of work has been directed toward the synthesis of new derivatives of piperidine because they can act as anticancer drugs (Varvaresou *et al.*, 1996), highly active serotonergic agents (Radl *et al.*, 1999) and other clinical medicines (Orjales *et al.*, 1995). However, to our knowledge, structural studies in this interesting area are quite rare. Since knowledge of the stereochemistry is so useful in the rational design of pharmaceuticals, we report herein the synthesis and X-ray crystal structure of the title compound, (I), as part of our effort to develop new functional compounds.



(I)

In (I), the piperidine ring takes a normal chair conformation, as shown in Fig. 1. Each phenolic group forms an intramolecular O—H···N hydrogen bond with the N-donor of the piperidine ring (Fig. 2) which may stabilize the structure.

Experimental

The title compound was prepared by the reaction of piperidine (2.42 g, 28.5 mmol), 2-*tert*-butyl-4-methylphenol (4.67 g, 28.4 mmol) and paraformaldehyde (0.85 g, 28.3 mmol) in ethanol (50 ml) at reflux for 4 h under argon. The reaction mixture was cooled and the white solid obtained was recrystallized from CH_2Cl_2/CH_3OH producing colorless single crystals suitable for X-ray diffraction. Yield: 95%; m.p.: 359–360 K. Analysis calculated for the title compound: C 78.11, H 10.41, N 5.36%; found: C 78.05, H 10.55, N 5.30%. ^{1}H NMR (CD_3COCD_3, δ, p.p.m.): 1.36 [*s*, 9H, $C(CH_3)_3$], 1.45 (*m*, 2H, CH_2), 1.62 (*m*, 4H, $2CH_2$), 2.19 (*s*, 3H, CH_3), 2.66 (*m*, 4H,

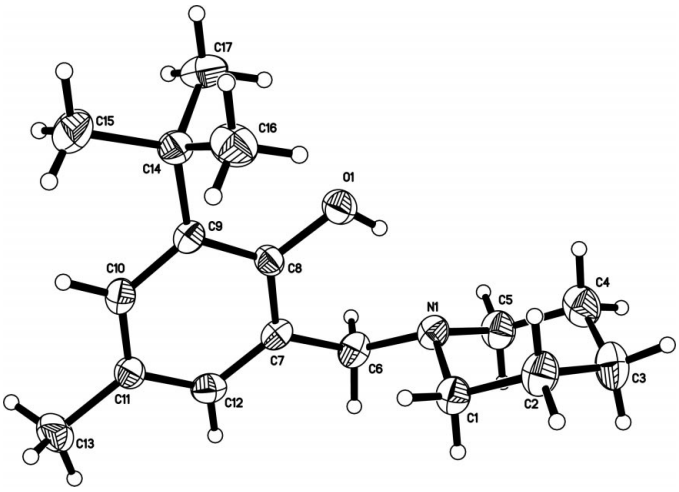


Figure 1
*ORTEP*II (Johnson, 1976) view of (I) shown with 30% probability ellipsoids.

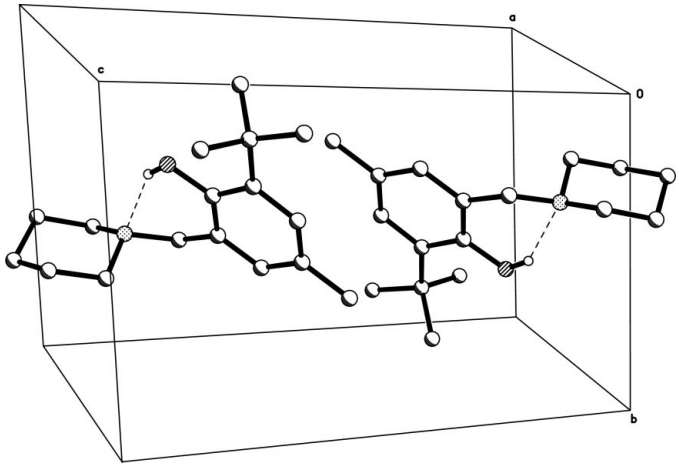


Figure 2
The unit-cell contents of (I).

2 CH_2), 3.61 (*s*, 2H, CH_2), 6.64 (*s*, 1H, ArH), 6.92 (*s*, 1H, ArH), 11.4 (*s*, 1H, OH).

Crystal data

$C_{17}H_{27}NO$
M_r = 261.40
Triclinic, $P\overline{1}$
a = 6.2854 (19) Å
b = 8.626 (3) Å
c = 15.318 (5) Å
α = 97.391 (6)°
β = 97.498 (6)°
γ = 100.559 (7)°
V = 799.5 (4) Å^3
Z = 2
D_x = 1.086 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3312 reflections
θ = 1.4–25.0°
μ = 0.07 mm^{-1}
T = 293 (2) K
Prism, colorless
0.25 × 0.20 × 0.20 mm

Data collection

Bruker SMART 1000 diffractometer
ω scans
Absorption correction: multi-scan [*SAINT* (Bruker, 1998) and *SADABS* (Sheldrick, 1997)]
T_{min} = 0.984, T_{max} = 0.987
3376 measured reflections
2818 independent reflections
1219 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 25.0°
$h = -6 \rightarrow 7$
$k = -7 \rightarrow 10$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.155
S = 0.99
2818 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.0223P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.022
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.457 (4)	N1—C6	1.466 (4)
N1—C5	1.464 (3)	O1—C8	1.372 (3)
C1—N1—C5	110.9 (2)	O1—C8—C7	119.5 (3)
C1—N1—C6	111.4 (2)	O1—C8—C9	118.7 (3)
C5—N1—C6	110.5 (2)	C7—C8—C9	121.7 (3)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···N1	0.82	1.95	2.660 (3)	145

All H-atom positions were calculated and included in subsequent refinement in a riding-model approximation.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART* (Bruker, 1998); data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS*-97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Bruker, 1998)

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