

erythro-2-Piperidinyl-1,2-diphenylethanol

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Key indicators

Single-crystal X-ray study

$T = 183$ K

Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å

R factor = 0.058

wR factor = 0.136

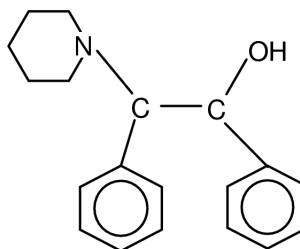
Data-to-parameter ratio = 20.1

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

The molecule of the title compound, $\text{C}_{19}\text{H}_{23}\text{NO}$, contains two phenyl rings and a piperidinyl ring. The dihedral angle between the phenyl rings is $40.99(5)^\circ$. The piperidine ring has a chair conformation. There is an intramolecular $\text{O}-\text{H}\cdots\text{N}$ hydrogen bond.

Comment

During the process of UV-radiation curing, oxygen is present as a free radical in the medium. To overcome the negative effect caused by the oxygen, we synthesized *erythro*-2-piperidinyl-1,2-diphenylethanol to use it as a hydrogen donor for Type II initiators (Davidson, 1999). In this paper we report the structure of *erythro*-2-piperidinyl-1,2-diphenylethanol, (I). An ORTEPIII (Burnett & Johnson, 1996) plot of the structure is shown in Fig. 1.



(I)

The C6–N1 and C1–N1 bond distances are 1.4749 (19) and 1.4730 (18) Å, respectively, and are similar to the corresponding bond lengths in ethyl 4-[2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy]benzoate [1.467 (5) and 1.472 (4) Å; Jottier *et al.*, 1991] and 3-[2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl]-2,9-dimethyl-4*H*-pyrido[1,2-*a*]pyrimidin-4-one (Ocaperidone) [1.477 (9) and 1.463 (9) Å; Jottier *et al.*, 1992]. The C7–N1, C7–C14 and C14–O2 bond distances are 1.4872 (17) 1.5563 (19) and 1.4286 (17) Å, respectively, similar to the corresponding bond lengths in *N*-(2-hydroxyethyl)-piperidine, *N*-(2-hydroxyethyl)morpholine and *N*-(2-hydroxyethyl)piperazine [1.495 (4), 1.493 (4) and 1.397 (4) Å, respectively; Castellari & Sabatino, 1996]. The *erythro*-2-piperidinyl-1,2-diphenylethanol molecule contains three rings: two phenyl rings and a piperidinyl ring. For the piperidinyl ring we calculated, following the method of Cremer & Pople (1975), phase angle $\theta_2 = 2.15(17)^\circ$ and $\varphi_2 = 34(5)^\circ$, indicating a chair conformation, and a puckering amplitude $Q = 0.5814(17)$ Å.

There is an intramolecular O2–H2A \cdots N1 hydrogen bond (Table 1).

Experimental

1 g of *trans*-stilbene oxide and 1 molar equivalent of distilled piperidine were refluxed for 12 h with vigorous stirring. The product was extracted with diethyl ether and excess morpholine was separated by the addition of 5 ml of distilled water. The combined organic layers were washed with distilled water several times. The solution was dried over anhydrous magnesium sulfate. The crude product was recrystallized from ethanol. M.p: 373 K Analysis calculated for C₁₉H₂₃NO: C, 81.14; H, 8.18; N, 4.98. Found C, 81.22; H, 8.19; N, 5.03.

Crystal data

C ₁₉ H ₂₃ NO	$D_x = 1.174 \text{ Mg m}^{-3}$
$M_r = 281.38$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 5874 reflections
$a = 13.6624 (10) \text{ \AA}$	$\theta = 3.0\text{--}28.3^\circ$
$b = 5.6452 (10) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$c = 20.678 (4) \text{ \AA}$	$T = 183 (2) \text{ K}$
$\beta = 93.46 (4)^\circ$	Block, colourless
$V = 1591.9 (4) \text{ \AA}^3$	$0.72 \times 0.50 \times 0.36 \text{ mm}$
$Z = 4$	

Data collection

Siemens SMART CCD area-detector diffractometer	2344 reflections with $I > 2\sigma(I)$
ω scans	$R_{\text{int}} = 0.080$
Absorption correction: none	$\theta_{\text{max}} = 28.3^\circ$
9095 measured reflections	$h = -15 \rightarrow 18$
3833 independent reflections	$k = -7 \rightarrow 7$
	$l = -27 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2)]$
$R[F^2 > 2\sigma(F^2)] = 0.058$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.136$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.81$	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
3833 reflections	$\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$
191 parameters	Extinction correction: <i>SHELXL</i>
H-atom parameters constrained	Extinction coefficient: 0.044 (4)

Table 1

Selected geometric parameters (\AA , $^\circ$).

O2—C14	1.4286 (17)	N1—C7	1.4872 (17)
N1—C1	1.4730 (18)	C7—C14	1.5563 (19)
N1—C6	1.4749 (19)		
C1—N1—C6	108.77 (12)	C8—C7—C14	110.26 (11)
C1—N1—C7	111.98 (11)	C9—C8—C13	117.81 (14)
C6—N1—C7	111.87 (11)	C9—C8—C7	122.51 (13)
N1—C6—C4	111.82 (13)	O2—C14—C15	109.76 (12)
N1—C7—C8	112.18 (11)	O2—C14—C7	109.39 (11)
N1—C7—C14	108.24 (11)		

Table 2

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

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O2—H2A \cdots N1	0.82	2.39	2.774 (2)	109

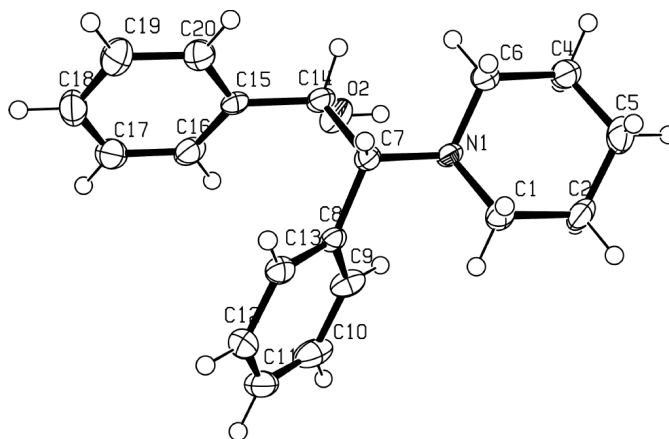


Figure 1

An ORTEP (Burnett & Johnson, 1996) drawing of the title compound, showing the atom-numbering scheme. Displacement ellipsoids of non-H atoms are shown at the 50% probability level.

All H atoms, located in a difference Fourier map, were positioned geometrically and constrained with a riding model. The C—H bond distances range from 0.93 to 0.98 \AA .

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 1990).

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