

## 1,17-Heptadecanediol

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In the title compound, C<sub>17</sub>H<sub>36</sub>O<sub>2</sub>, one of the hydroxyl groups has a *gauche* conformation with respect to the hydrocarbon skeleton, which is all-*trans*, whereas the other has a *trans* conformation. The molecular shape is rod-like and the compound has a rotator phase in which molecules are assured greater motional freedom, as in liquid crystals. In addition, the molecules arranged along the longest axis, *b*, form layers which are very similar to those of the smectic A liquid crystals.

## Comment

The crystallographic investigation of long-chain organic molecules has been ongoing since the early days of X-ray crystallography; for example, early work on paraffins (Müller, 1928) demonstrated the rod-like conformation of these molecules in the crystalline state. The structures of nine  $\alpha,\omega$ -alkanediols containing 10–16, 18 and 21 C atoms have been investigated recently as models for polymers and/or smectic liquid crystals by Nakamura and his co-workers: 1,10-decanediol (Nakamura & Sato, 1999*a*), 1,11-undecanediol (Nakamura *et al.*, 1999), 1,12-dodecanediol (Nakamura & Setodoi, 1997), 1,13-tridecanediol (Nakamura *et al.*, 1997), 1,14-tetradecanediol (Nakamura & Sato, 1999*b*), 1,15-pentadecanediol (Nakamura, Uno, Watanabe *et al.*, 2000), 1,16-hexadecanediol (Nakamura & Yamamoto, 1994), 1,18-octadecanediol (Nakamura & Watanabe, 2001) and 1,21-henicosanediol (Nakamura, Uno & Ogawa, 2000). The results showed a consistent distinction between the structures with even and odd numbers of C atoms. In the  $\alpha,\omega$ -alkanediols with an even number of C atoms, the hydroxyl groups showed an all-*trans* conformation with respect to the skeleton. In these structures, the molecules are arranged in layers in a herringbone fashion similar to smectic C liquid crystals. In contrast, in the structures of the  $\alpha,\omega$ -alkanediols with an odd number of C atoms, one hydroxyl group adopts a *gauche* conformation with respect to the hydrocarbon skeleton, whereas the other hydroxyl group adopts a *trans* conformation. In these structures, the molecules form a layer structure which is similar to that found in smectic A liquid crystals. In addition, phase

transitions in  $\alpha,\omega$ -alkanediols with C<sub>13</sub>–C<sub>24</sub> were studied and a linear relation between the longest unit-cell length and number of C atoms was reported using powder X-ray diffraction (Ogawa & Nakamura, 1999).

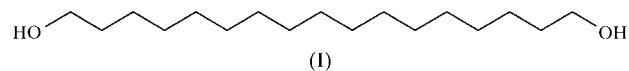
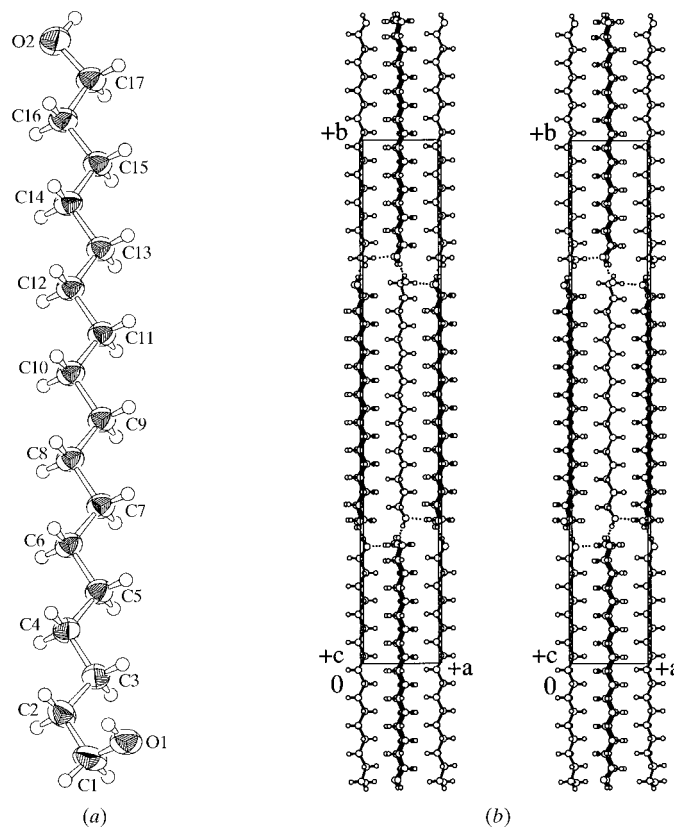


Fig. 1(*a*) shows the molecular structure of 1,17-heptadecanediol, (I). Except for the length of the *b* axis, the longest axis, no appreciable differences are observed between the crystal data obtained in this study and those of the homologues with odd numbers of C atoms reported previously. The terminal torsion angles O1–C1–C2–C3 and O2–C17–C16–C15 are 63.3 (3) and  $-179.3$  (2)°, respectively. This means that the former has a *gauche* conformation and the latter a *trans* conformation. The existence of a *gauche* conformation in the molecules is a typical feature of the structures of  $\alpha,\omega$ -alkanediols with an odd number of C atoms. The molecules are arranged along the *b* axis forming layers with a thickness of *a*/2, as can be seen in Fig. 1(*b*). It should be noted that this layer structure is quite similar to the smectic A structure of liquid crystals. This structure of (I), as well as those of the homologues with an odd number of C atoms, has two different types of hydrogen bond, *i.e.* interlayer and intralayer. The donor–acceptor distances of interlayer and intralayer hydrogen bonds are 2.782 (4) and 2.705 (2) Å,



**Figure 1**  
(*a*) An ORTEPII (Johnson, 1976) view of the title molecule showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. (*b*) A stereoview of the crystal structure projected along the *c* axis. Dotted lines indicate the hydrogen bonding.

respectively. The values of torsion angles of the *gauche* conformation observed in this study are in good agreement with those of other  $\alpha,\omega$ -alkanediol structures containing an odd number of C atoms [e.g. 1,11-undecanediol 63.3 (3)°, 1,15-pentadecanediol 63.2 (4)° and 1,21-henicosanediol 65.1 (5)°]. The distances of both hydrogen bonds are also comparable to those of 1,11-undecanediol [2.775 (3) and 2.710 (2) Å], 1,13-tridecanediol [2.776 (4) and 2.713 (2) Å], 1,15-pentadecanediol [2.777 (3) and 2.713 (2) Å] and 1,21-henicosanediol [2.778 (4) and 2.717 (3) Å].

The above observations contrast with the structures of  $\alpha,\omega$ -alkanediols with an even number of C atoms. The all-*trans* structures contain only one type of hydrogen bond. The centrosymmetric molecules are arranged in a zigzag manner adopting a herring-bone motif. This kind of structure had been observed not only in  $\alpha,\omega$ -alkanediols with an even number of C atoms but also in several examples of  $\alpha,\omega$ -alkanediol-bromides: 1,12-dibromododecane (Kupke *et al.*, 1981), 1,16-dibromohexadecane (Kobayashi *et al.*, 1995) and 1,18-dibromooctadecane (Nakamura *et al.*, 1993). All these structures are similar to the smectic C structure of liquid crystals.

## Experimental

The title compound was synthesized as described previously (Ogawa & Nakamura, 1999). The single crystal used for analysis was grown by slow evaporation from a solution containing a mixture of methanol, ethyl acetate and *n*-heptane (1:1:3).

### Crystal data

$C_{17}H_{36}O_2$	Cu $K\alpha$ radiation
$M_r = 272.47$	Cell parameters from 24 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 9.3\text{--}16.2^\circ$
$a = 7.197$ (4) Å	$\mu = 0.496$ mm <sup>-1</sup>
$b = 47.756$ (2) Å	$T = 296.2$ K
$c = 5.076$ (3) Å	Plate, colorless
$V = 1744$ (1) Å <sup>3</sup>	$0.80 \times 0.40 \times 0.02$ mm
$Z = 4$	
$D_x = 1.037$ Mg m <sup>-3</sup>	

### Data collection

Rigaku AFC-5R diffractometer	$R_{int} = 0.043$
$\omega$ scans	$\theta_{max} = 70.57^\circ$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$h = -2 \rightarrow 8$
$T_{min} = 0.882$ , $T_{max} = 0.999$	$k = -1 \rightarrow 58$
3140 measured reflections	$l = -1 \rightarrow 6$
1929 independent reflections	3 standard reflections
1335 reflections with $I > 2\sigma(I)$	every 150 reflections
	intensity decay: 1.41%

### Refinement

Refinement on $F$	H atoms treated by a mixture of independent and constrained refinement
$R = 0.044$	$w = 1/[\sigma^2(F_o) + 0.00063 F_o ^2]$
$wR = 0.054$	$(\Delta/\sigma)_{max} = 0.0004$
$S = 1.459$	$\Delta\rho_{max} = 0.13$ e Å <sup>-3</sup>
1335 reflections	$\Delta\rho_{min} = -0.21$ e Å <sup>-3</sup>
180 parameters	

The methylene H atoms were located at idealized positions, and were allowed to ride on the parent C atoms (C—H = 0.97 Å). The H-atom isotropic displacement parameters were set to be  $1.2U_{eq}$  of the parent C atom. The hydroxyl H atoms were located from a difference Fourier map, and were allowed to refine isotropically for the final refinements [O—H = 0.84 (3) and 0.87 (3) Å].

**Table 1**

Selected geometric parameters (Å, °).

O1—C1	1.424 (3)	C8—C9	1.518 (3)
O2—C17	1.423 (3)	C9—C10	1.517 (3)
C1—C2	1.501 (3)	C10—C11	1.515 (3)
C2—C3	1.514 (3)	C11—C12	1.514 (3)
C3—C4	1.516 (3)	C12—C13	1.517 (3)
C4—C5	1.512 (3)	C13—C14	1.517 (3)
C5—C6	1.520 (3)	C14—C15	1.516 (3)
C6—C7	1.517 (3)	C15—C16	1.519 (3)
C7—C8	1.516 (3)	C16—C17	1.507 (3)
O1—C1—C2	112.8 (2)	C9—C10—C11	114.3 (2)
C1—C2—C3	115.0 (2)	C10—C11—C12	113.8 (2)
C2—C3—C4	112.9 (2)	C11—C12—C13	114.6 (2)
C3—C4—C5	114.9 (2)	C12—C13—C14	113.8 (2)
C4—C5—C6	113.5 (2)	C13—C14—C15	114.8 (2)
C5—C6—C7	114.2 (2)	C14—C15—C16	112.4 (2)
C6—C7—C8	113.6 (2)	C15—C16—C17	114.0 (2)
C7—C8—C9	114.2 (2)	O2—C17—C16	108.6 (2)
C8—C9—C10	113.9 (2)		
O1—C1—C2—C3	63.3 (3)	O2—C17—C16—C15	-179.3 (2)

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1992); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1995); program(s) used to solve structure: *SAPI91* (Fan, 1991); program(s) used to refine structure: *TEXSAN*; software used to prepare material for publication: *TEXSAN*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: BJ1023). Services for accessing these data are described at the back of the journal.

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