

## 1,15-Pentadecanediol

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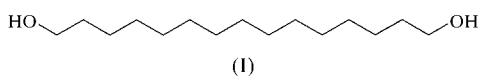
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In the title compound, C<sub>15</sub>H<sub>32</sub>O<sub>2</sub>, one of the terminal hydroxyl groups has a *gauche* conformation with respect to the hydrocarbon skeleton, while the other is *trans*. The molecules lie parallel to the longest axis and form layers similar to those of the smectic A structure of liquid crystals. These features are similar to those of the homologues with an odd number of C atoms, but different from those with an even number.

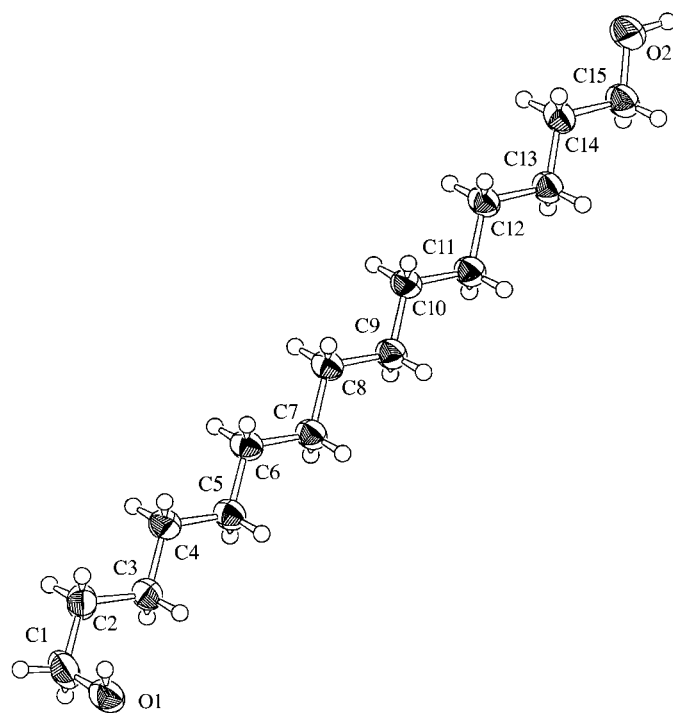
## Comment

Normal long-chain compounds have attracted attention as a basic model of polymers, as they have a very simple chemical structure whose molecular skeleton is a straight hydrocarbon chain. In addition, these compounds have a layer structure similar to the smectic one of liquid crystals, and could therefore be regarded as the model compound of liquid crystals. Many researchers have studied crystal structures of normal long-chain compounds, for example, *n*-alkanes (Müller, 1928) and  $\alpha$ -monosubstituted *n*-alkanes, such as *n*-higher alcohols (e.g. Watanabe, 1961; Seto, 1962). Recently, some of the present authors reported phase-transition phenomena of normal long-chain  $\alpha,\omega$ -alkanediols from C<sub>13</sub> to C<sub>24</sub> (Ogawa & Nakamura, 1999). Crystal structures of six  $\alpha,\omega$ -alkanediols, namely 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*) and 1,16-hexadecanediol (Nakamura & Yamamoto, 1994), have also been reported.



The molecular structure of 1,15-pentadecanediol, (I), is shown in Fig. 1. The essential structural parameters and shape of the molecule are quite similar to those of the homologues with an odd number of C atoms already reported, except for the *b*-axis lattice parameter. The terminal C1—O1 bond has a

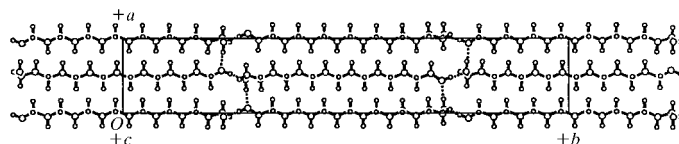
*gauche* conformation with respect to the skeleton [O1—C1—C2—C3 torsion angle of 63.2 (4)<sup>o</sup>], whereas the other terminal C15—O2 bond is *trans* [O2—C15—C14—C13 torsion angle of −179.2 (2)<sup>o</sup>]. The molecules lie parallel to the *b* axis, forming layers with a thickness of *b*/2. The molecules are arranged in an antiparallel fashion along the *a* axis in these layers, as can be seen in Fig. 2. This packing is very similar to the smectic A structure of liquid crystals. In this structure, the molecules form two different types of hydrogen bond, *i.e.* interlayer and intralayer hydrogen bonds. These features are already found in the homologues with an odd number of C atoms. The interlayer and intralayer O1...O2 hydrogen-bond distances are 2.713 (2) and 2.777 (3) Å, respectively. The values of the hydrogen-bond distance are in good agreement with those of 1,11-undecanediol [2.710 (2) and 2.775 (3) Å] and 1,13-tridecanediol [2.713 (2) and 2.776 (4) Å].



**Figure 1**

An ORTEP (Johnson, 1976) view of the title molecule showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

In our previous papers, we reported that the molecular and crystal structures of the homologues with an even number of C atoms (1,10-decanediol, 1,12-dodecanediol, 1,14-tetradecanediol and 1,16-hexadecanediol) are different from those of the homologues with an odd number of C atoms. The hydrocarbon skeleton had the all-*trans* conformation, and both terminal C—O bonds also showed the *trans* conformation. The centrosymmetric molecules are arranged in a zigzag manner to make a herring-bone motif. The structure could be regarded as a model structure of the smectic C liquid crystals. 1,12-Dibromododecane (Kupke *et al.*, 1981), 1,16-dibromohexadecane (Kobayashi *et al.*, 1995) and 1,18-dibromooctadecane (Nakamura *et al.*, 1993) also showed the herring-bone motif. In these structures, only interlayer hydrogen bonds are found.



**Figure 2**  
The projection of the crystal structure of the title molecule along the *c* axis. Dotted lines indicate the hydrogen bond.

## Experimental

According to the conventional method, the title compound was synthesized from commercially available pentadecanedioic acid (Tokyo Kasei Kogyo Co. Ltd) by esterification and reduction with  $\text{LiAlH}_4$ . The single crystal used for analysis was grown by very slow evaporation from a solution in a mixed solvent system consisting of methanol, ethyl acetate and *n*-heptane (1:1:3).

### Crystal data

$\text{C}_{15}\text{H}_{32}\text{O}_2$	Cu $K\alpha$ radiation
$M_r = 244.42$	Cell parameters from 25 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 35.4\text{--}38.9^\circ$
$a = 7.177(2) \text{ \AA}$	$\mu = 0.508 \text{ mm}^{-1}$
$b = 42.670(2) \text{ \AA}$	$T = 296.2 \text{ K}$
$c = 5.090(2) \text{ \AA}$	Plate, colourless
$V = 1559.0(8) \text{ \AA}^3$	$0.6 \times 0.30 \times 0.030 \text{ mm}$
$Z = 4$	
$D_x = 1.041 \text{ Mg m}^{-3}$	

### Data collection

Rigaku AFC-5R diffractometer	$R_{\text{int}} = 0.029$
$\omega$ - $2\theta$ scans	$\theta_{\text{max}} = 70.59^\circ$
Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968)	$h = -2 \rightarrow 8$
$T_{\text{min}} = 0.917$ , $T_{\text{max}} = 0.999$	$k = 0 \rightarrow 52$
2756 measured reflections	$l = -1 \rightarrow 6$
1734 independent reflections	3 standard reflections
1165 reflections with $I > 2\sigma(I)$	every 150 reflections
	intensity decay: 8.80%

### Refinement

Refinement on $F$	H-atom parameters not refined
$R = 0.049$	$w = 1/[\sigma^2(F_o) + 0.00063 F_o ^2]$
$wR = 0.058$	$(\Delta/\sigma)_{\text{max}} = 0.0004$
$S = 1.516$	$\Delta\rho_{\text{max}} = 0.14 \text{ e \AA}^{-3}$
1165 reflections	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
154 parameters	

All H atoms, including hydroxyl H atoms, were fixed in idealized positions.

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:

**Table 1**

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

O1—C1	1.422 (4)	C7—C8	1.512 (3)
O2—C15	1.419 (3)	C8—C9	1.517 (3)
C1—C2	1.497 (4)	C9—C10	1.516 (3)
C2—C3	1.515 (3)	C10—C11	1.515 (3)
C3—C4	1.513 (3)	C11—C12	1.517 (3)
C4—C5	1.511 (3)	C12—C13	1.519 (3)
C5—C6	1.519 (3)	C13—C14	1.514 (3)
C6—C7	1.516 (3)	C14—C15	1.502 (3)
O1—C1—C2	112.7 (2)	C8—C9—C10	113.8 (2)
C1—C2—C3	115.2 (3)	C9—C10—C11	114.5 (2)
C2—C3—C4	113.2 (2)	C10—C11—C12	113.5 (2)
C3—C4—C5	115.0 (2)	C11—C12—C13	115.0 (2)
C4—C5—C6	113.7 (2)	C12—C13—C14	112.9 (2)
C5—C6—C7	114.6 (2)	C13—C14—C15	114.3 (2)
C6—C7—C8	113.8 (2)	O2—C15—C14	108.6 (2)
C7—C8—C9	114.4 (2)		
O1—C1—C2—C3	63.2 (4)	O2—C15—C14—C13	−179.2 (2)

*TEXSAN*; software used to prepare material for publication: *TEXSAN*.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DE1141). Services for accessing these data are described at the back of the journal.

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