(3S)-3-Benzyloxyethyl-1,4-dioxane-2,5-dione

The lactide ring in the title compound, \( \text{C}_{12}\text{H}_{12}\text{O}_{5} \), adopts a screw-boat conformation. C–H...O interactions link the molecules into a chain in the [100] direction.

Comment

The structure of the title compound, (I), was determined in the course of our investigations towards a better understanding of the regioselectivity observed in the ring-opening polymerization of various substituted (3S)-3-benzyloxyethyl-1,4-dioxane-2,5-dione derivatives (Leemhuis et al., 2005). Earlier, we reported the crystal structures of the 6(R)-methyl (Kooijman et al., 2005a) and the 6(S)-methyl derivatives (Kooijman et al., 2005b). The molecular structure of (I) is displayed in Fig. 1 and selected geometric parameters are given in Table 1.

The lactide ring has taken a somewhat deformed screw-boat conformation. The asymmetry parameter (Duax & Norton, 1975) \( \Delta C_{2}(C_{2}–O_{3}) = 6.4 (5) \); all other asymmetry parameters have values of 18\(^\circ\) or higher. The Cremer & Pople puckering parameters (Cremer & Pople, 1975) are \( \theta = \)

**Figure 1**

Atomic displacement plot (Spek, 2003) of the title compound, showing the atom-numbering scheme. The displacement ellipsoids are drawn at the 50% probability level.
77.1 (6)° and ϕ = 320.3 (6)°; the ideal values for the observed screw-boat conformation are θ = 67.5° and ϕ = 330°. The benzyloxymethyl substituent of the lactide ring occupies the axial position, as illustrated by the angle between the least-squares plane through the non-planar lactide ring and the C5—C6 bond, which amounts to 77.9 (3)°. In the 6(R)-methyl derivative, the benzyloxymethyl group also occupies the axial position [plane–bond angle = 67.20 (13)°]. The 6(S)-methyl derivative, however, has the benzyloxymethyl group in the equatorial position [plane–bond angle = 13.13 (13)°], most likely due to steric hindrance between the substituents of the lactide ring. The link between the two ring systems is not in an all-trans conformation, the torsion angles C4—C5—C6—O4 and O5—C7—C8—C9 having the gauche conformation.

The packing displays short C–H⋯O contacts, geometric details of which are given in Table 2. These contacts link the molecules into an infinite chain in the [100] direction (see Fig. 2).

**Experimental**

The synthesis of the title compound is described elsewhere (Leemhuis et al., 2003). Crystals were grown from a solution in methyl tert-butyl ether.

**Crystal data**

C12H12O5, Mr = 236.22

Monoclinic, P21

α = 6.925 (4) Å

b = 7.025 (4) Å

c = 11.733 (8) Å

β = 103.44 (3)°

V = 555.2 (6) Å³

Z = 2

**Data collection**

Nonius KappaCCD area-detector diffractometer

899 reflections with I > 2σ(I)

θmax = 25.3°

S = 1.11

1098 reflections

154 parameters

H-atoms parameters constrained

**Refinement**

Refinement on F²

wR(F²) = 0.102

S = 1.11

1098 reflections

154 parameters

In the absence of significant anomalous scatterers, Friedel’s law still holds. Friedel pairs were therefore averaged. The absolute configuration of C5 was chosen in accordance with the enanitopure starting material. H atoms were introduced in calculated positions, with C–H = 0.95–1.00 Å, and refined as riding on their carrier atoms, with Uiso(H) = 1.2Uiso(C).

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997); data reduction: DENZO; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: PLATON.

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**References**


