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1-*O*-*p*-Toluenesulfonyl-2,3:4,5-di-*O*-isopropylidene-L-arabitol

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Key indicators

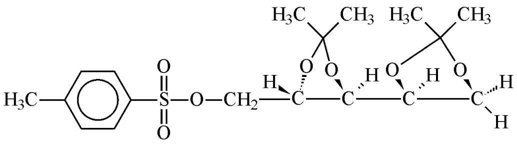
Single-crystal X-ray study
T = 143 K
Mean σ(C–C) = 0.003 Å
R factor = 0.040
wR factor = 0.100
Data-to-parameter ratio = 17.3

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

In the title compound, $C_{18}H_{26}SO_7$, the absolute configuration was confirmed as S at all three chiral centres. Molecules are linked by three C—H···O contacts.

Comment

The title compound, (I), is a representative of a class of compounds important in the synthesis of polyhydroxyalkyl derivatives (Holy, 1978, 1982).



(I)

The molecule of (I) is shown in Fig. 1. The absolute configuration is confirmed as S at all three chiral centres C2, C3 and C4.

The conformation of the five-membered ring C2/C3/C10/O8/C9 is approximately twist (local diad through O9 and the midpoint of C3—O8) and that of C4/C5/C13/O6/C7 is approximately envelope (local mirror though C4 and the midpoint of C13—O6).

Molecules are linked by three C—H···O contacts that may be regarded as weak hydrogen bonds (Table 2); one, H4···O17, is much shorter than the others. The two contacts with purely translational symmetry operators link the molecules to form layers parallel to the ac plane at $y \simeq \frac{1}{4}, \frac{3}{4}$ (Fig. 2).

Experimental

The title compound was synthesized starting from L-arabitol, as described by Holy (1982). Single crystals were formed when the mother liquor was left undisturbed.

Crystal data

$C_{18}H_{26}O_7S$
M_r = 386.45
Monoclinic, $P2_1$
a = 7.9957 (10) Å
b = 14.527 (3) Å
c = 8.3194 (14) Å
β = 94.93 (2)°
V = 962.8 (3) Å^3
Z = 2
D_x = 1.333 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 52 reflections
θ = 10–11.5°
μ = 0.20 mm^{-1}
T = 143 (2) K
Plate, colourless
0.70 × 0.50 × 0.15 mm

Data collection

Stoe Stadi4 diffractometer
ω/θ scans
Absorption correction: none
4605 measured reflections
4154 independent reflections
3891 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.018
$\theta_{\rm max}$ = 27.5°
$h = -10 \rightarrow 10$
$k = -16 \rightarrow 18$
$l = -10 \rightarrow 10$
3 standard reflections
frequency: 60 min
intensity decay: 1.3%

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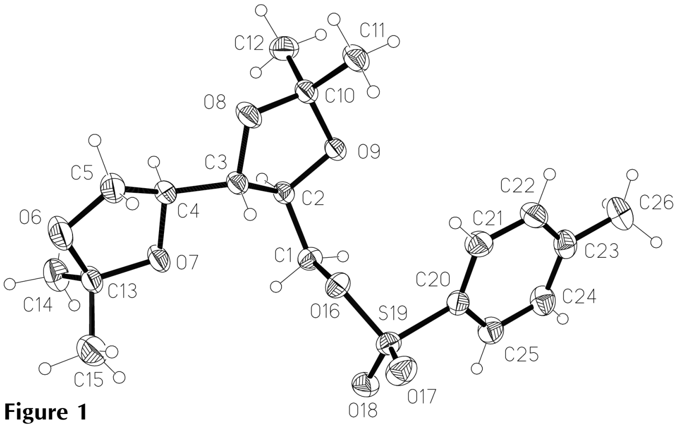

Figure 1
The molecule of the title compound, (I), in the crystal. Displacement ellipsoids are drawn at the 50% probability level. H-atom radii are arbitrary.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.100$
$S = 1.04$
4154 reflections
240 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.2455P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.23$ e Å^{-3}
$\Delta\rho_{\min} = -0.24$ e Å^{-3}
Absolute structure: Flack (1983)
Flack parameter = 0.01 (7)

Table 1
Selected torsion angles (Å).

O9—C2—C3—O8	29.19 (19)	C3—C2—O9—C10	−37.49 (19)
O7—C4—C5—O6	−33.0 (2)	C2—O9—C10—O8	31.7 (2)
C4—C5—O6—C13	24.3 (2)	C3—O8—C10—O9	−12.0 (2)
C5—C4—O7—C13	30.2 (2)	C4—O7—C13—O6	−16.1 (2)
C2—C3—O8—C10	−10.7 (2)	C5—O6—C13—O7	−6.2 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···O17$^{\rm i}$	1.00	2.48	3.396 (3)	152
C15—H15C···O8$^{\rm ii}$	0.98	2.61	3.509 (3)	153
C24—H24···O17$^{\rm iii}$	0.95	2.63	3.521 (3)	156

Symmetry codes: (i) $x, y, 1+z$; (ii) $-x, \frac{1}{2}+y, 2-z$; (iii) $1+x, y, z$.

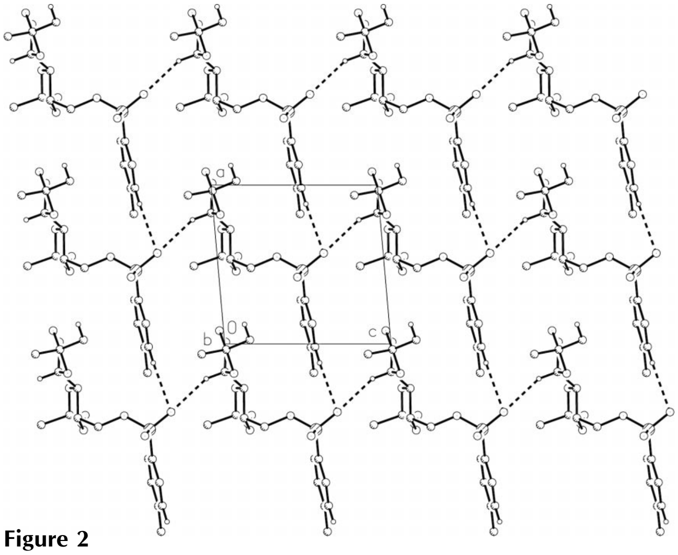

Figure 2
Packing diagram of (I), projected parallel to the b axis. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonds have been omitted.

Methyl H atoms were identified in difference syntheses, idealized and then refined using rigid methyl groups (C—H = 0.98 Å and H—C—H = 109.5°) allowed to rotate but not tip. Other H atoms were included using a riding model, with C—H = 0.95 (sp^2), 0.99 (methylene) or 1.00 Å (methine). The absolute configuration was based on 1849 Friedel pairs.

Data collection: *DIF*4 (Stoe & Cie, 1992); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL*97.

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