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Benzyl 4-*C*-nitrosomethyl-*β*-D-arabinopyranoside

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean *σ*(C–C) = 0.005 Å
R factor = 0.058
wR factor = 0.052
Data-to-parameter ratio = 8.9

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

The title compound [systematic name: (2*R*,3*S*,4*S*,5*R*)-2-(benzyloxy)-5-(nitromethyl)-3,4,5,6-tetrahydro-2*H*-pyran-3,4,5-triol], $C_{13}H_{17}NO_7$, has the nitrosomethyl group in the equatorial position. The bond lengths and angles are as expected.

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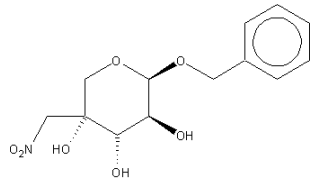
Comment

Benzyl 4-*C*-nitrosomethyl *β*-D-arabinopyranoside, $C_{13}H_{17}NO_7$, is one of the intermediates in the synthesis of isofagomine from benzyl *β*-D-*threo*-pent-1-4-diuloside (Andersch & Bols, 2001). The structure was determined to confirm that the compound had the required configuration, with the nitrosomethyl group in the equatorial position, before continuing with the synthesis. The bond lengths and angles are as expected. Intermolecular hydrogen bonds link the molecules in chains along the *b* axis.



(I)

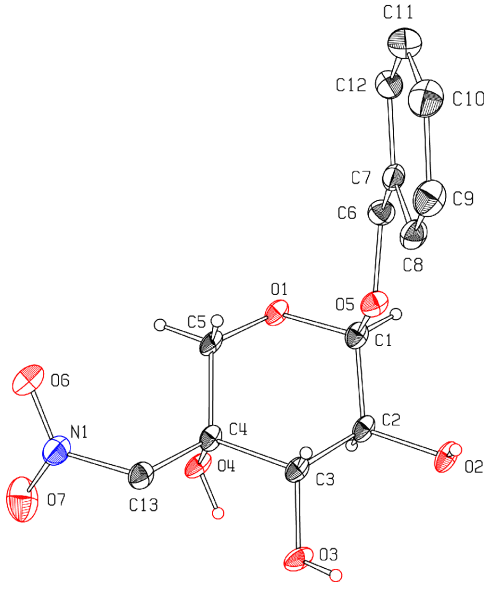


Figure 1
View of the molecule, showing the labelling of the non-H atoms. Displacement ellipsoids are drawn at the 50% probability level. H atoms of the sugar ring are shown as small circles of arbitrary radii, while those of the phenyl ring have been omitted.

Experimental

Crystal data

$C_{13}H_{17}NO_7$
$M_r = 299.28$
Monoclinic, $P2_1$
$a = 11.497\ (3)$ Å
$b = 5.538\ (1)$ Å
$c = 11.603\ (3)$ Å
$\beta = 117.792\ (5)^\circ$
$V = 653.5\ (3)$ Å^3
$Z = 2$
$D_x = 1.521$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2950 reflections
$\theta = 2.1$–30.0°
$\mu = 0.12$ mm^{-1}
$T = 120$ K
Needle, colourless
0.50 × 0.10 × 0.05 mm

Data collection

Siemens SMART CCD diffractometer
ω scans
8029 measured reflections
1781 independent reflections
1692 reflections with $I > 0.01$
$R_{int} = 0.136$
$\theta_{max} = 28.3^\circ$
$h = -15 \rightarrow 15$
$k = -7 \rightarrow 7$
$l = -15 \rightarrow 15$

Refinement

Refinement on F
$R = 0.058$
$wR = 0.052$
$S = 0.99$
1692 reflections
190 parameters
H-atom parameters constrained
$w = 1/\{[\sigma_{cs}(F^2 + B) + (1+A)F^2]^{1/2} - |F|\}^2$ where $A = 0.03$ and $B = 1.0$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43\ (10)$ e Å^{-3}
$\Delta\rho_{min} = -0.35\ (10)$ e Å^{-3}
Extinction correction: B–C type 1 Lorentzian isotropic (Becker & Coppens, 1974)
Extinction coefficient: 120 (16)

In the absence of significant anomalous scattering, Friedel pairs have been merged. The absolute configuration cannot be established from the diffraction data and has been assumed from the synthesis. The positions of the H atoms of the hydroxy groups were determined from a difference map and were kept fixed; the other H atoms were constrained to have C—H = 0.95 Å and $U_{iso} = 1.2U_{eq}$(C).

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SIR*97 (Altomare *et al.*, 1997) and *KRYSTAL* (Hazell, 1995); program(s) used to refine structure: modified *ORFLS* (Busing *et al.*, 1962) and *KRYSTAL*; molecular graphics: *ORTEP*III (Burnett & Johnson, 1996) and *KRYSTAL*; software used to prepare material for publication: *KRYSTAL*.

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