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## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.034  
 $wR$  factor = 0.086  
Data-to-parameter ratio = 7.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

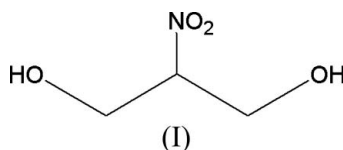
## 2-Nitropropane-1,3-diol

The title molecule,  $\text{C}_3\text{H}_7\text{NO}_4$ , adopts a nearly symmetric conformation. The crystal structure is stabilized by intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, linking the molecules to form a three-dimensional framework.

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## Comment

The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation. We report here the synthesis and the crystal structure of (I).



In the molecule of (I) (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The  $\text{C}1-\text{C}3/\text{O}3/\text{O}4$  and  $\text{C}2/\text{N}1/\text{O}1/\text{O}2$  groups are each planar, with maximum deviations of 0.0435 (3) Å (C3) and 0.0009 (2) Å (N1) from the least-squares planes, respectively. They form a dihedral angle of 86.12 (3)°.

It is well known that nitro substituents are very strong electron-withdrawing groups, so the  $\text{C}1-\text{C}2-\text{C}3$  [113.3 (2)°] angle is enlarged. On the other hand, the electron-withdrawing character of the nitro group has an influence on the  $\text{C}2-\text{N}1$  [1.496 (3) Å] bond length, as in *N*-(*p*-nitrophenylsulfonyl)-1*H*-pyrrole (Gültekin *et al.*, 2004).

As can be seen from the packing diagram (Fig. 2), intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 1) link the molecules to form a three-dimensional framework. Dipole-dipole and van der Waals interactions are also effective in the molecular packing in the crystal structure.

## Experimental

Paraformaldehyde (51.0 g, 1700.0 mmol) and potassium carbonate (0.3 g, 2.2 mmol) were added to a solution of nitromethane (30.5 g, 500.0 mmol) in absolute methyl alcohol (470 ml). The mixture was heated on a steam-bath until the formaldehyde had disappeared, and then it was heated for an additional 10 min. The solution of the triol 2-hydroxymethyl-2-nitropropane-1,3-diol was cooled to 273 K and the flask fitted with a stirrer and a dropping funnel. A solution of sodium methylate, which had been prepared from sodium (14.0 g 608.7 mmol) and absolute methyl alcohol (245 ml), was added dropwise during the course of 0.5 h, while the mixture was stirred and kept at 273 K. The mixture was maintained at 273 K for 2 h. The precipitated sodium derivative of the diol was filtered and washed

with cold methyl alcohol. A solution, prepared from salicylic acid (24.8 g, 179.7 mmol) and diethyl ether (400 ml), was refluxed and the sodium derivative (41.4 g, 200.0 mmol) added during the course of 0.5 h. After the mixture had been refluxed for 1.5 h, the precipitated sodium salicylate was removed and the solvent distilled under reduced pressure. The residue was cooled and the crystalline product pressed free from oil (yield 55%, m.p. 327 K). Single crystals of the title compound were obtained by slow evaporation of a solution in ethyl acetate/chloroform (1:1.7).

#### Crystal data

$C_3H_7NO_4$	$Z = 4$
$M_r = 121.10$	$D_x = 1.445 \text{ Mg m}^{-3}$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 10.331(3) \text{ \AA}$	$\mu = 0.14 \text{ mm}^{-1}$
$b = 6.322(2) \text{ \AA}$	$T = 294(2) \text{ K}$
$c = 8.520(3) \text{ \AA}$	Prism, colorless
$V = 556.5(3) \text{ \AA}^3$	$0.24 \times 0.20 \times 0.18 \text{ mm}$

#### Data collection

Bruker SMART CCD area-detector diffractometer	2868 measured reflections
$\varphi$ and $\omega$ scans	597 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	505 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.968$ , $T_{\max} = 0.976$	$R_{\text{int}} = 0.027$
	$\theta_{\max} = 26.2^\circ$

#### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0499P)^2 + 0.0466P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.086$	$(\Delta/\sigma)_{\max} < 0.001$
$S = 1.07$	$\Delta\rho_{\max} = 0.12 \text{ e \AA}^{-3}$
597 reflections	$\Delta\rho_{\min} = -0.14 \text{ e \AA}^{-3}$
79 parameters	
H atoms treated by a mixture of independent and constrained refinement	

**Table 1**

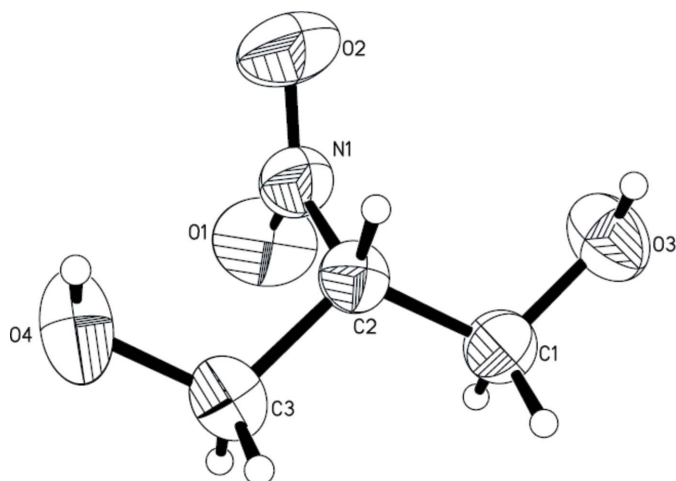
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O4-H4\cdots O3^i$	0.92 (5)	1.88 (5)	2.765 (3)	161 (4)
$O3-H3\cdots O4^{ii}$	0.85 (5)	1.97 (5)	2.800 (3)	165 (4)

Symmetry codes: (i)  $-x + \frac{3}{2}, y - \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $x - \frac{1}{2}, -y + \frac{3}{2}, z$ .

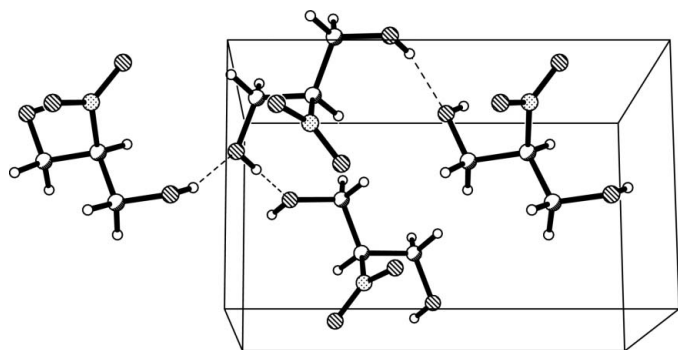
The hydroxyl H atoms were located in difference syntheses, and refined [ $O-H = 0.85(5)$  and  $0.92(5) \text{ \AA}$ ;  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ ]. The remaining H atoms were positioned geometrically, with  $C-H = 0.98$  and  $0.97 \text{ \AA}$  for methine and methylene H atoms, respectively, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine



**Figure 1**

A plot of the title molecule structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**

A partial packing diagram of (I). Intermolecular  $O-H\cdots O$  hydrogen bonds are shown as dashed lines.

structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1997); software used to prepare material for publication: SHELXTL.

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