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## Key indicators

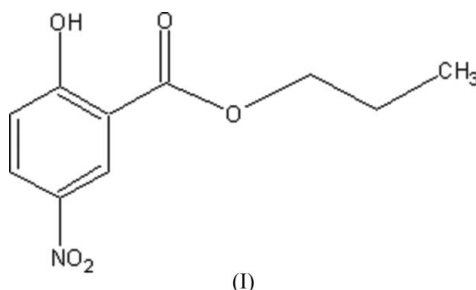
Single-crystal X-ray study  
 $T = 292$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å  
 $R$  factor = 0.056  
 $wR$  factor = 0.166  
Data-to-parameter ratio = 15.6For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## 1-Propyl 5-nitrosalicylate

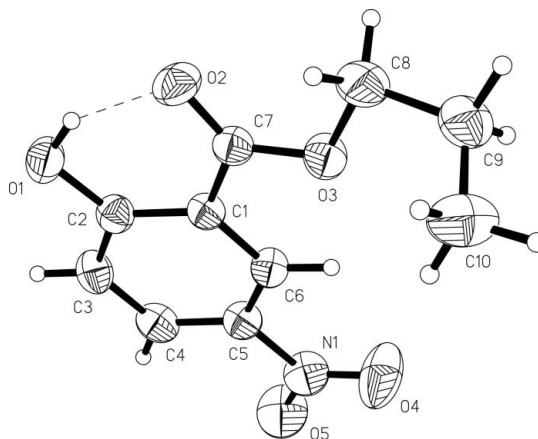
In the title compound,  $\text{C}_{10}\text{H}_{11}\text{NO}_5$ , all bond lengths and angles show normal values. Weak intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds form centrosymmetric dimers, which are further linked by  $\pi-\pi$  interactions into ladders extending along the  $a$  axis.

## Comment

Many compounds in the salicylate series exhibit a broad range of biological activities (Yuan & Tsao, 1994) and other useful properties (Liu *et al.*, 1996). These derivatives may serve as ligands, coordinating to metal ions through the ester group. As a part of our study of biologically active esters and their complexes (Jin *et al.*, 2004; Jin & Xiao, 2005), we present the crystal structure of the title compound, (I) (Fig. 1).



The bond lengths and angles in (I) show normal values (Table 1). An intramolecular hydrogen bond is observed between the hydroxyl group and the O atom of the carbonyl group (Table 2). In the crystal structure, weak intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 2) form centrosymmetric



**Figure 1**  
The molecular structure of (I), showing 30% probability displacement ellipsoids and the intramolecular hydrogen bond (dashed line).

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dimers (Fig. 2). Within the dimer, an  $O2 \cdots O2(-x, -y, 1-z)$  short contact of 2.763 (3) Å is observed. The dimers are stacked with  $\pi$ - $\pi$  interactions, as shown by the short  $O1 \cdots C7^{ii}$  contact of 3.182 (3) Å [symmetry code (ii):  $1-x, -y, 1-z$ ], thus forming ladders extending along the  $a$  axis.

## Experimental

Compound (I) was synthesized according to the literature procedure of Bartlett & Trachtenberg (1958). A crystal suitable for X-ray analysis was grown from a solution in ethanol at room temperature by slow evaporation.

### Crystal data

$C_{10}H_{11}NO_5$	$D_x = 1.393 \text{ Mg m}^{-3}$
$M_r = 225.20$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 626 reflections
$a = 5.1084$ (8) Å	$\theta = 2.9$ – $19.6^\circ$
$b = 11.5966$ (18) Å	$\mu = 0.11 \text{ mm}^{-1}$
$c = 18.166$ (3) Å	$T = 292$ (2) K
$\beta = 94.018$ (3)°	Block, colourless
$V = 1073.5$ (3) Å <sup>3</sup>	$0.20 \times 0.16 \times 0.10 \text{ mm}$
$Z = 4$	

### Data collection

Bruker SMART APEX CCD area-detector diffractometer	2346 independent reflections
$\varphi$ and $\omega$ scans	1086 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.046$
$T_{\text{min}} = 0.978$ , $T_{\text{max}} = 0.989$	$\theta_{\text{max}} = 27.0^\circ$
6263 measured reflections	$h = -6 \rightarrow 6$
	$k = -14 \rightarrow 14$
	$l = -21 \rightarrow 23$

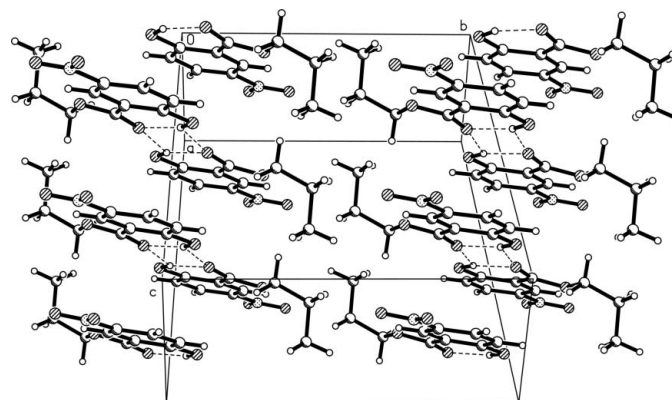
### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.056$	$w = 1/[\sigma^2(F_o^2) + (0.0695P)^2]$
$wR(F^2) = 0.166$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2346 reflections	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
150 parameters	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

C1–C7	1.467 (3)	C7–O3	1.325 (3)
C2–O1	1.343 (3)	C8–O3	1.459 (3)
C5–N1	1.468 (4)	N1–O4	1.208 (3)
C7–O2	1.214 (3)	N1–O5	1.213 (3)
O1–C2–C1	123.1 (2)	C10–C9–C8	114.6 (3)
O2–C7–O3	122.9 (2)	O4–N1–O5	122.9 (3)
O2–C7–C1	122.9 (2)	C2–O1–H1	105 (2)
O3–C8–C9	108.0 (2)	C7–O3–C8	115.9 (2)
C6–C1–C2–O1	−179.2 (2)	C6–C5–N1–O5	−176.4 (3)
C7–C1–C2–O1	0.9 (4)	O2–C7–O3–C8	−2.0 (4)
C4–C5–N1–O4	−176.0 (3)	C1–C7–O3–C8	178.1 (2)



**Figure 2**

A packing diagram for (I). Hydrogen bonds are indicated by dashed lines.

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1–H1 $\cdots$ O2	0.94 (4)	1.77 (4)	2.619 (3)	149 (3)
O1–H1 $\cdots$ O2 <sup>i</sup>	0.94 (4)	2.37 (4)	3.045 (3)	129 (3)

Symmetry codes: (i)  $-x, -y, -z + 1$ .

The hydroxyl H atom was located in a difference Fourier map and refined isotropically, with  $O-H = 0.94$  (4) Å. All other H atoms were positioned geometrically and refined as riding, with  $C-H$  distances of 0.93 (aromatic H), 0.96 (methyl H) and 0.97 Å (methylene H), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic and methylene H, or  $1.5U_{\text{eq}}(\text{C})$  for methyl H.

Data collection: SMART APEX (Bruker, 2001); cell refinement: SMART APEX; data reduction: SAINT-Plus (Bruker, 2001); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-NT (Bruker, 2001); software used to prepare material for publication: SHELXTL-NT.

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