IUCrData

ISSN 2414-3146

Propyl 4-aminobenzoate

Alexander J. Gutzwiller, Christine K. F. Hermann and George N. Harakas*

PO Box 6949, Radford University, Radford, Virginia 24142, USA. *Correspondence e-mail: gharakas@radford.edu

Received 28 April 2026
Accepted 30 April 2026

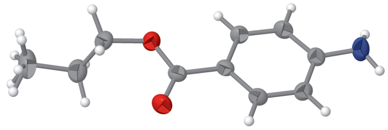
Keywords: crystal structure; hydrogen bonding.

CCDC reference: 2550860

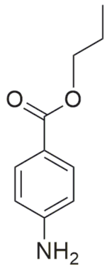
Structural data: full structural data are available from iucrdata.iucr.org

The structure of the title compound, $C_{10}H_{13}NO_2$, shows the *n*-propyl group to be perpendicular to the remaining part of the molecule; carboxylate-C—O—C—C(*n*-propyl) torsion angle = −87.05 (19)°. In the crystal, amine-N—H···O(carbonyl) and weaker amine-N—H···N(amine) hydrogen bonding occurs within double layers parallel to the *ab* plane. The hydrogen atoms of the methyl group are disordered over two sets of sites in the ratio 0.89 (3) to 0.11 (3).

3D view



Chemical scheme



Structure description

The reaction of 4-aminobenzoic acid with 1-propanol yielded the title compound *n*-propyl 4-aminobenzoate (risocaine). Risocaine, its isomer, isopropyl 4-aminobenzoate, and amines with similar structures have medical applications such as pain relievers (Priyanka *et al.*, 2022).

The crystal structure we report complements the physical and spectroscopic data collected as part of a guided inquiry undergraduate Organic Chemistry laboratory experiment (Hermann *et al.*, 2026). In this guided inquiry experiment, students synthesized and characterized solid esters, selected for ease of purification and handling. Students were provided with a list of possible carboxylic acids and alcohols but not the specific reactants assigned to each group. After synthesis, they compared the observed melting point range of their product to a reference table. Furthermore, students recorded the IR, ^{1}H NMR, and ^{13}C NMR spectra of their product to confirm their conclusions from the melting point range.

Referring to Fig. 1, the C9 atom of the *n*-propyl group is close to perpendicular to the carboxylate residue as seen in the C7—O1—C8—C9 torsion angle of −87.05 (19)°. The equivalent torsion angles for one of the terminal –CH_3 groups in isopropyl 4-aminobenzoate (two independent molecules) are −77.8 (4) and −86.5 (4)°, while the other –CH_3 groups approach coplanarity, *i.e.* 159.5 (3) and 152.5 (4)° (Priyanka *et al.*, 2022). The carboxylate [the C2—C1—C7—O2 torsion angle = 176.86 (17)°] and amine

https://doi.org/10.1107/S2414314626004566

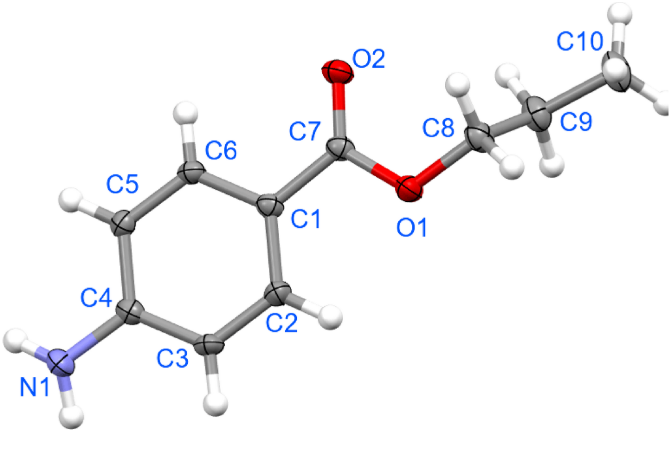


Figure 1
The molecular structure of the title compound showing displacement ellipsoids at the 30% probability level. Only the major component of the disordered hydrogen atoms on C10 are shown.

[C2—C3—C4—N1 = 174.94 (17)°] groups are close to coplanar to the benzene ring to which they are connected.

The molecular packing (Fig. 2) shows hydrogen-bonding interactions between the amine functional group and the carbonyl group of the ester and weaker amine-N—H···N(amine) hydrogen bonding; distances and angle are listed in Table 1. The hydrogen bonding occurs within double layers that stack along the *c* axis.

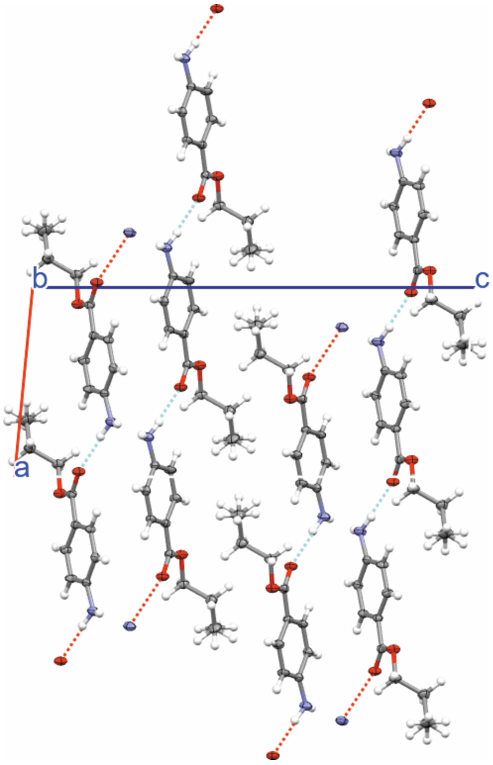


Figure 2
Crystal packing viewed along the *b* axis. Hydrogen-bonding interactions are shown as dashed lines.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N1^{i}	0.88 (2)	2.55 (2)	3.397 (3)	162 (2)
N1—H1B···O2^{ii}	0.88 (2)	2.09 (2)	2.964 (2)	173 (2)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{10}H_{13}NO_2$
M_r	179.21
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	233
a, b, c (Å)	8.5011 (3), 5.8300 (2), 19.7631 (8)
β (°)	95.453 (2)
V (Å^3)	975.05 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.41 × 0.21 × 0.21
Data collection	
Diffractometer	Bruker D8
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.966, 0.982
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	37794, 2427, 2283
R_{int}	0.039
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.668
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.159, 1.17
No. of reflections	2427
No. of parameters	126
No. of restraints	5
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.39, −0.27

Computer programs: *APEX3* and *SAINT* (Bruker, 2019), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/2* (Sheldrick, 2015*b*) and *ShelXle* (Hübschle *et al.*, 2011).

Synthesis and crystallization

Referring to Fig. 3, the title compound was synthesized through a Fischer esterification. A mixture of 4-aminobenzoic acid (1.5 g), 1-propanol (10 ml), and concentrated sulfuric acid (1 ml) was refluxed in a 50 ml boiling flask for 1 h. The reaction mixture was allowed to cool; a solution of 10% sodium carbonate was added until a pH of 8 was obtained. The solution was chilled in an ice bath until a solid product was formed. The solid was isolated by vacuum filtration.

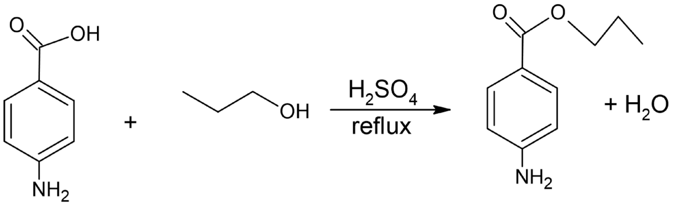


Figure 3
Reaction scheme for the title compound.

The yield was 0.864 grams (57.0%) with a melting point of 72.7°C, which compared to a literature value of 73–75°C. The IR and NMR spectra confirmed the structure (Hermann *et al.*, 2026).

X-ray quality crystals were produced by dissolving the product into methanol, followed by adding an equal volume of hexanes. The solvent was allowed to evaporate over several days. A single-crystal was coated with NVH oil and mounted on a MiTeGen loop then cooled to −40 °C for data collection.

Refinement

Crystal data, data collection, and structure refinement details are summarized in Table 2. The hydrogen atoms on the methyl-C10 atom are disordered over two positions and refined to a 0.89 (3) to 0.11 (3) occupancy ratio.

References

Bruker (2019). *APEX3* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Hermann, C. K. F., Gutzwiller, A., Addison, G. & Turner, B. (2026). *Engaging Students in Organic Chemistry* vol. 2, ch. 7, pp. 91–101. ACS Symposium Series, vol. 1521. https:/doi.org/10.1021/bk-2026-1521.ch007.

Hübschle, C. B., Sheldrick, G. M. & Dittrich, B. (2011). *J. Appl. Cryst.* **44**, 1281–1284.

Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.

Priyanka, P., Jayanna, B. K., Kiran Kumar, H., Yathirajan, H. S., Divakara, T. R., Foro, S. & Butcher, R. J. (2022). *IUCrData* **7**, x220904.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2026). **11**, x260456 [https://doi.org/10.1107/S2414314626004566]

Propyl 4-aminobenzoate

Alexander J. Gutzwiller, Christine K. F. Hermann and George N. Harakas

Propyl 4-aminobenzoate

Crystal data

$C_{10}H_{13}NO_2$
M_r = 179.21
Monoclinic, $P2_1/n$
a = 8.5011 (3) Å
b = 5.8300 (2) Å
c = 19.7631 (8) Å
β = 95.453 (2)°
V = 975.05 (6) Å^3
Z = 4
F(000) = 384
D_x = 1.221 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9986 reflections
θ = 3.7–28.3°
μ = 0.09 mm^{-1}
T = 233 K
Block, colourless
0.41 × 0.21 × 0.21 mm

Data collection

Bruker D8 diffractometer
Radiation source: sealed tube
Flat graphite monochromator
Detector resolution: 7.391 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{\min}$ = 0.966, $T_{\max}$ = 0.982
37794 measured reflections
2427 independent reflections
2283 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
$\theta_{\max}$ = 28.3°, $\theta_{\min}$ = 3.7°
$h = -11 \rightarrow 11$
$k = -7 \rightarrow 7$
$l = -26 \rightarrow 26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.159
S = 1.17
2427 reflections
126 parameters
5 restraints
Primary atom site location: Intrinsic Phasing
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0557P)^2 + 0.6285P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.39 e Å^{-3}
$\Delta\rho_{\min}$ = −0.27 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.41184 (15)	0.7084 (2)	0.39339 (8)	0.0407 (4)	
O2	0.52677 (15)	0.3933 (2)	0.35610 (7)	0.0420 (4)	
N1	−0.21045 (19)	0.1716 (3)	0.29235 (10)	0.0450 (4)	
H1A	−0.220 (3)	0.028 (3)	0.2790 (13)	0.068*	
H1B	−0.287 (2)	0.229 (4)	0.3145 (13)	0.068*	
C1	0.24626 (19)	0.4106 (3)	0.35136 (8)	0.0300 (4)	
C2	0.1139 (2)	0.5332 (3)	0.36787 (10)	0.0362 (4)	
H2	0.127429	0.673133	0.391334	0.043*	
C3	−0.0363 (2)	0.4507 (3)	0.35001 (10)	0.0389 (4)	
H3	−0.124141	0.534562	0.361780	0.047*	
C4	−0.0597 (2)	0.2444 (3)	0.31471 (9)	0.0324 (4)	
C5	0.0731 (2)	0.1194 (3)	0.29957 (9)	0.0327 (4)	
H5	0.059756	−0.022164	0.276956	0.039*	
C6	0.2229 (2)	0.2018 (3)	0.31749 (9)	0.0320 (4)	
H6	0.310763	0.116125	0.306731	0.038*	
C7	0.4082 (2)	0.4970 (3)	0.36686 (9)	0.0313 (4)	
C8	0.5655 (2)	0.8188 (3)	0.40383 (11)	0.0403 (4)	
H8A	0.551542	0.985495	0.400907	0.048*	
H8B	0.629878	0.771708	0.367673	0.048*	
C9	0.6508 (2)	0.7587 (4)	0.47167 (11)	0.0471 (5)	
H9A	0.680761	0.596304	0.472127	0.057*	
H9B	0.580694	0.783509	0.507594	0.057*	
C10	0.7985 (3)	0.9069 (5)	0.48517 (14)	0.0621 (7)	
H10A	0.866055	0.885591	0.448792	0.093*	0.89 (3)
H10B	0.855180	0.862316	0.528067	0.093*	0.89 (3)
H10C	0.768012	1.066875	0.487229	0.093*	0.89 (3)
H10D	0.793444	0.990931	0.527267	0.093*	0.11 (3)
H10E	0.804318	1.014205	0.447992	0.093*	0.11 (3)
H10F	0.891486	0.809646	0.488829	0.093*	0.11 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0293 (6)	0.0326 (7)	0.0598 (9)	0.0002 (5)	0.0014 (6)	−0.0065 (6)
O2	0.0275 (6)	0.0401 (8)	0.0582 (9)	0.0056 (5)	0.0037 (6)	−0.0025 (6)
N1	0.0287 (8)	0.0482 (10)	0.0585 (11)	−0.0060 (7)	0.0061 (7)	−0.0119 (9)
C1	0.0271 (8)	0.0291 (8)	0.0336 (8)	0.0033 (6)	0.0022 (6)	0.0025 (7)
C2	0.0315 (8)	0.0311 (9)	0.0457 (10)	0.0040 (7)	0.0017 (7)	−0.0074 (8)
C3	0.0270 (8)	0.0363 (10)	0.0538 (11)	0.0090 (7)	0.0054 (7)	−0.0077 (8)
C4	0.0273 (8)	0.0354 (9)	0.0344 (8)	0.0002 (7)	0.0035 (6)	0.0025 (7)
C5	0.0347 (9)	0.0290 (8)	0.0345 (8)	0.0001 (7)	0.0040 (7)	−0.0042 (7)
C6	0.0278 (8)	0.0311 (9)	0.0375 (9)	0.0057 (7)	0.0051 (6)	−0.0016 (7)
C7	0.0295 (8)	0.0299 (8)	0.0344 (8)	0.0032 (7)	0.0021 (6)	0.0042 (7)
C8	0.0355 (9)	0.0317 (9)	0.0534 (11)	−0.0063 (8)	0.0025 (8)	0.0034 (8)
C9	0.0427 (11)	0.0492 (12)	0.0489 (11)	−0.0090 (9)	0.0010 (9)	0.0010 (9)

C10	0.0493 (13)	0.0730 (17)	0.0619 (14)	−0.0224 (12)	−0.0059 (10)	−0.0058 (13)

Geometric parameters (Å, º)

O1—C7	1.338 (2)	C2—C3	1.379 (3)
O1—C8	1.453 (2)	C3—C4	1.395 (3)
O2—C7	1.212 (2)	C4—C5	1.400 (2)
N1—C4	1.382 (2)	C5—C6	1.376 (2)
C1—C6	1.394 (2)	C8—C9	1.504 (3)
C1—C2	1.398 (2)	C9—C10	1.527 (3)
C1—C7	1.470 (2)		
C7—O1—C8	116.80 (14)	C3—C4—C5	118.45 (16)
C6—C1—C2	118.51 (16)	C6—C5—C4	120.56 (16)
C6—C1—C7	119.17 (15)	C5—C6—C1	121.01 (16)
C2—C1—C7	122.30 (16)	O2—C7—O1	122.63 (16)
C3—C2—C1	120.55 (17)	O2—C7—C1	124.79 (17)
C2—C3—C4	120.88 (16)	O1—C7—C1	112.57 (14)
N1—C4—C3	120.56 (16)	O1—C8—C9	111.97 (16)
N1—C4—C5	120.92 (17)	C8—C9—C10	110.04 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N1$^{\rm i}$	0.88 (2)	2.55 (2)	3.397 (3)	162 (2)
N1—H1*B*···O2$^{\rm ii}$	0.88 (2)	2.09 (2)	2.964 (2)	173 (2)

Symmetry codes: (i) $-x-1/2, y-1/2, -z+1/2$; (ii) $x-1, y, z$.