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(4*SR*)-4-Benzyl-4-hydroxyisoxazolidin-3-one

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The title compound, $C_{10}H_{11}NO_3$, was synthesized by the reaction of ethyl 3-aminoxy-2-benzyl-2-hydroxypropanoate with potassium hydroxide. It was found to crystallize with two independent molecules in the asymmetric unit. In the crystal structure, O—H···O and N—H···O interactions link the molecules into one-dimensional chains along the crystallographic *a* axis.

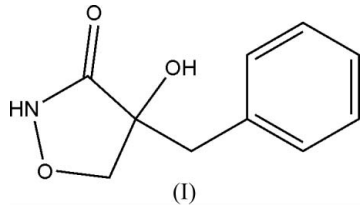
Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.004 Å
R factor = 0.043
wR factor = 0.106
Data-to-parameter ratio = 8.4

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

Comment

Tabtoxinine-β-lactam is a natural compound, which inhibits glutamine synthetase, causing chlorosis and death of tobacco plants. In order to synthesize this compound by a new method, a model compound, 3-benzyl-3-hydroxyazetidin-2-one, has been designed. The title compound, (I), is a precursor for this model.



(I)

The asymmetric unit of (I) contains two independent molecules (Fig. 1). The dihedral angles between the phenyl planes (C5–C10 and C15–C20) and the isoxazolidine rings (C1/C2/C3/N1/O2 and C11/C12/C13/N2/O5) are 50.0 (5) and 49.3 (4)°, respectively. Considering the crystal packing, O—H···O and N—H···O hydrogen bonds link neighbouring molecules into one-dimensional chains along the [100] direction (Table 1 and Fig. 2). Further analysis of the crystal packing suggests that there are some weak C—H···O interactions stabilizing the packing of (I).

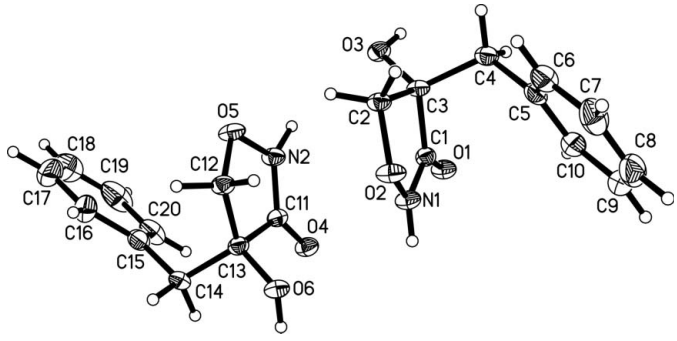


Figure 1
The asymmetric unit of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

Experimental

The title compound was prepared according to a published procedure (Pohland, 1955). Colourless platelet single crystals were obtained by recrystallization from methanol (m.p. 421 K). Analysis, found: C 62.37, H 5.56, N 7.33%; calculated for $C_{10}H_{11}NO_3$: C 62.17, H 5.74, N 7.25%.

Crystal data

$C_{10}H_{11}NO_3$
M_r = 193.20
Orthorhombic, $Pna2_1$
a = 7.8287 (8) Å
b = 7.8026 (8) Å
c = 30.6427 (18) Å
V = 1871.8 (3) Å^3
Z = 8
D_x = 1.371 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 113 (2) K
Plate, colourless
0.22 × 0.20 × 0.10 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.968, T_{max} = 0.990
13397 measured reflections
2246 independent reflections
2179 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.8°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.106
S = 1.08
2246 reflections
266 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 0.3587P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.018 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.84 (3)	1.94 (3)	2.786 (3)	176 (3)
O3—H3···O1^{ii}	0.84 (4)	1.97 (4)	2.813 (3)	177 (3)
N2—H2···O4^{ii}	0.99 (3)	1.80 (3)	2.784 (3)	170 (3)
O6—H6···O4^{i}	0.90 (4)	1.92 (4)	2.805 (3)	166 (3)

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

In the absence of significant anomalous dispersion effects, Friedel pairs were merged. H atoms bonded to heteroatoms were located in a difference map and their positional parameters were refined using a riding model, with U_{iso}(H) = 1.5U_{eq}(N,O). Other H atoms were positioned geometrically and refined using a riding model, with C—H bond lengths constrained to 0.95 (aromatic CH) or 0.99 Å (methylene CH_2), and U_{iso}(H) = 1.2U_{eq}(carrier C).

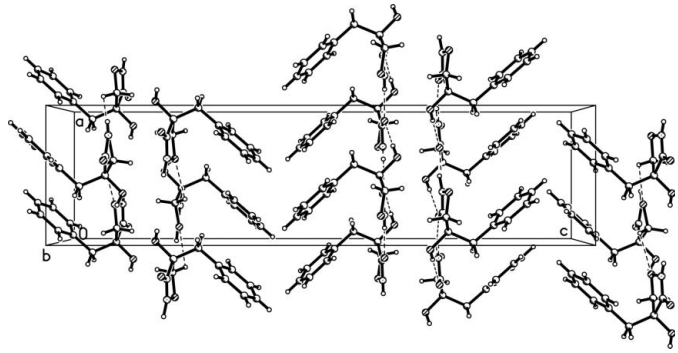


Figure 2
Packing diagram for (I) with hydrogen bonds drawn as dashed lines, as viewed along the [010] direction.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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