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(*S*,*S*)-2,2′-(1,2-Ethanediyldiimino)dibutan-1-ol

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.041
wR factor = 0.102
Data-to-parameter ratio = 9.3

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

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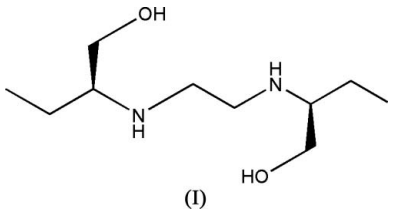
The title compound, $C_{10}H_{24}N_2O_2$, was synthesized by *N*-alkylation of 1,2-dichloroethane with (*S*)-2-amino-1-butanol. In the crystal structure, O—H···N and N—H···O link the molecules into sheets in the *bc* plane.

Comment

Ethambutol hydrochloride is a widely used chiral anti-tuberculosis agent (Fadnavis *et al.*, 1999). The title compound, (I), which is also called ethambutol, is the precursor of ethambutol hydrochloride and its structure is reported here (Fig. 1 and Table 1).



(I)

All bond lengths and angles in (I) are within normal ranges (Table 1; Allen *et al.*, 1987). The crystal structure is stabilized by intermolecular O—H···N and N—H···O hydrogen bonds which link the molecules into sheets in the *bc* plane (Fig. 2 and Table 2).

Experimental

The title compound was prepared according to the procedure of Bai *et al.* (2004). Colourless single crystals of (I) were grown by slow evaporation of a methanol solution.

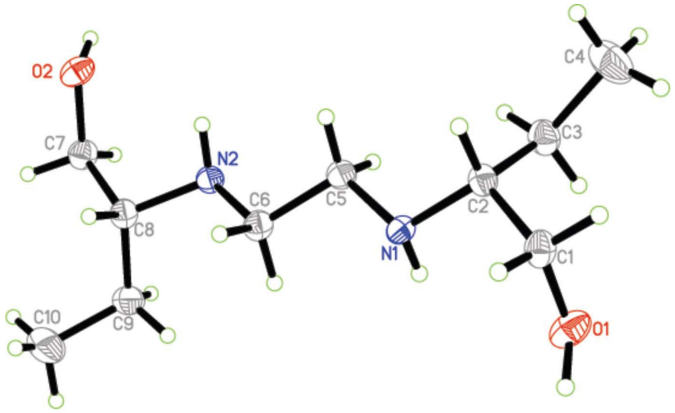


Figure 1
The molecular structure of (I), with the atom-numbering scheme and 30% probability displacement ellipsoids.

Crystal data

$C_{10}H_{24}N_2O_2$
$M_r = 204.31$
Monoclinic, $P2_1$
$a = 7.157$ (3) Å
$b = 8.440$ (4) Å
$c = 10.193$ (5) Å
$\beta = 95.631$ (8)°
$V = 612.7$ (5) Å^3
$Z = 2$
$D_x = 1.107$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 294$ (2) K
Block, colourless
0.22 × 0.20 × 0.10 mm

Data collection

Bruker SMART-1000 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.983$, $T_{max} = 0.992$
3317 measured reflections
1318 independent reflections
1049 reflections with $I > 2\sigma(I)$
$R_{int} = 0.026$
$\theta_{max} = 26.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.102$
$S = 1.07$
1318 reflections
141 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0537P)^2 + 0.0476P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.419 (3)		
C2—N1—C5	115.4 (2)	N1—C5—C6	109.7 (2)
N1—C2—C1	108.3 (2)		
O1—C1—C2—N1	61.4 (3)	N1—C5—C6—N2	−173.0 (2)
N1—C2—C3—C4	162.1 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.93 (5)	1.95 (5)	2.877 (3)	174 (3)
O2—H2B···N1^{ii}	0.96 (4)	1.82 (4)	2.767 (3)	174 (3)
N1—H1C···O2^{iii}	0.85 (3)	2.23 (3)	3.014 (3)	153 (3)

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

In the absence of significant anomalous dispersion effects, Freidel pairs were merged. The H atoms of the OH groups were initially located in a difference Fourier map and were restrained on their atoms with O—H restrained in the range 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(O). H atoms bonded to N atoms were refined independently with N—H restrained in the range of 0.85–0.90 Å and U_{iso}(H) = 1.2U_{eq}(N). Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.96–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl 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 structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

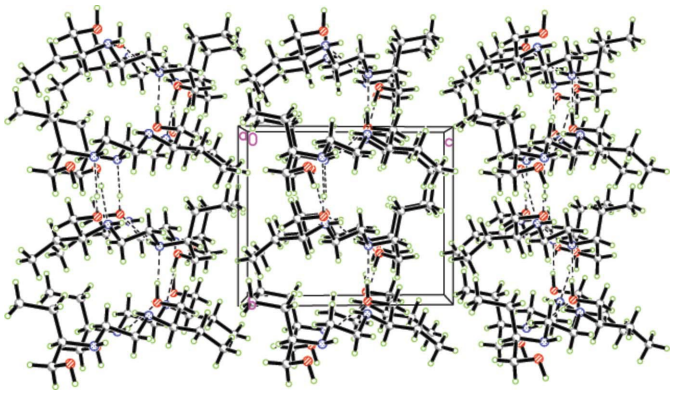


Figure 2
Packing diagram for (I), with hydrogen bonds shown as dashed lines.

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(*S*,*S*)-2,2′-(1,2-Ethanediyldiimino)dibutan-1-ol. Corrigendum

Guo-Yi Bai,[a]* Chen-Fang Zhang,[a] Yue-Cheng Zhang,[b] Tao Zeng[b] and Jiang-Sheng Li[b]

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In the paper by Bai, Zhang, Zhang, Zeng & Li [*Acta Cryst.* (2006), E**62**, o2173–o2174], the data relate to the *R*,*R* rather than the *S*,*S* enantiomer. The revised ellipsoid plot, packing diagram and selected geometrical data are given here.

Experimental

Data collection

R_{int} = 0.029

Refinement

$w = 1/[\sigma^2(F_o^2) + (0.0546P)^2 + 0.0456P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C1	1.419 (3)		
C2—N1—C5	115.4 (2)	N1—C5—C6	109.7 (2)
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N1—C2—C3—C4	−162.1 (3)		

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Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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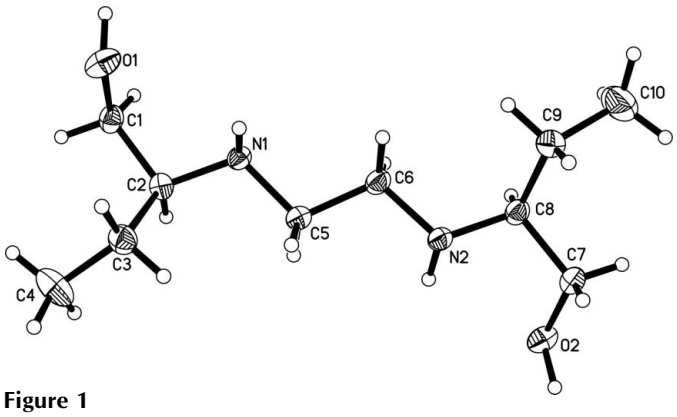
Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+1$; (ii) $2-x, y+\frac{1}{2}, -z+1$; (iii) $x-1, y, z$.



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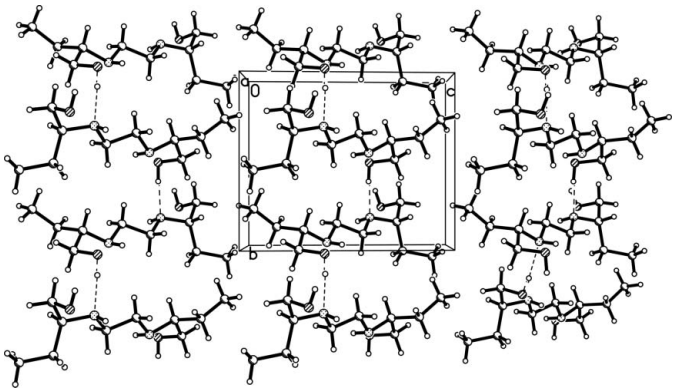

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