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(*R*,*S*)-2,2′-(Ethane-1,2-diyldiimino)dibutan-1-ol

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Key indicators

Single-crystal X-ray study
T = 113 K
Mean σ(C–C) = 0.002 Å
R factor = 0.059
wR factor = 0.130
Data-to-parameter ratio = 15.8

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

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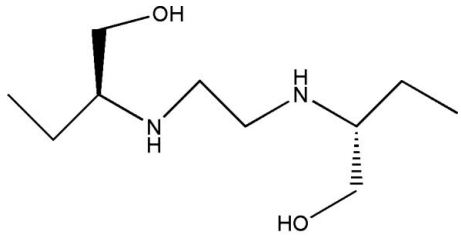
The title compound, $C_{10}H_{24}N_2O_2$, was synthesized by *N*-alkylation of 1,2-dichloroethane with racemic 2-amino-1-butanol. The molecule lies on a crystallographic inversion center and the crystal structure is stabilized by intermolecular O—H···N and N—H···O hydrogen bonds.

Comment

Ethambutol hydrochloride is a widely used chiral anti-tubercular agent (Fadnavis *et al.*, 1999). The title compound, (I), is the *meso* isomer of (*S*,*S*)-ethambutol (Bai *et al.*, 2006), a precursor of ethambutol hydrochloride.



(I)

The molecular structure of (I) is shown in Fig. 1. There is a center of inversion at the mid-point of the central C---C bond. All bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The crystal structure is stabilized by intermolecular O—H···N and N—H···O hydrogen bonds (Fig. 2 and Table 1).

Experimental

The title compound was prepared according to the procedure of Bai *et al.* (2004) using racemic 2-amino-1-butanol and 1,2-dichloroethane

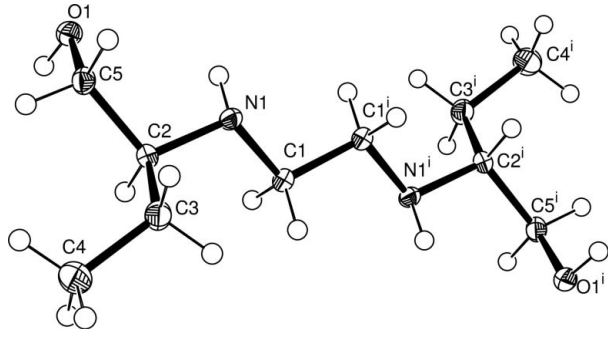


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids. [Symmetry code: (i) $-x$, $2-y$, $-x$.]

as reagents. Colorless single crystals were grown by slow evaporation of a methanol solution of (I).

Crystal data

$C_{10}H_{24}N_2O_2$
M_r = 204.31
Monoclinic, $P2_1/n$
a = 4.6334 (13) Å
b = 5.4777 (14) Å
c = 23.161 (2) Å
β = 95.336 (6)°
V = 585.3 (2) Å^3
Z = 2
D_x = 1.159 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 113 (2) K
Block, colorless
0.12 × 0.08 × 0.04 mm

Data collection

Rigaku Saturn diffractometer
ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.979, T_{max} = 0.997
5952 measured reflections
1157 independent reflections
1035 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.130
S = 1.20
1157 reflections
73 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0573P)^2 + 0.1608P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.90 (2)	2.33 (2)	3.163 (2)	152.9 (16)
N1—H1···O1	0.90 (2)	2.444 (19)	2.9051 (19)	112.1 (14)
O1—H6···N1^{ii}	0.87 (3)	1.95 (3)	2.810 (2)	172 (2)

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

H atoms bonded to N and O atoms were located in a difference Fourier map and refined isotropically. H atoms bonded to C atoms were positioned geometrically and refined using the riding-model approximation, with C—H = 0.99–1.00 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

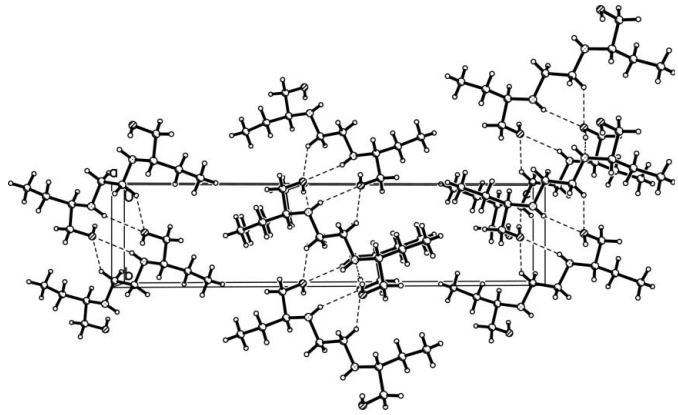


Figure 2
Part of the crystal structure of (I), with hydrogen bonds shown as dashed lines.

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: *CrystalStructure* (Rigaku/MSC, 2005); software used to prepare material for publication: *CrystalStructure*.

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