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1-(1,3-Benzothiazol-2-yl)propan-2-ol

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.118
Data-to-parameter ratio = 17.4

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

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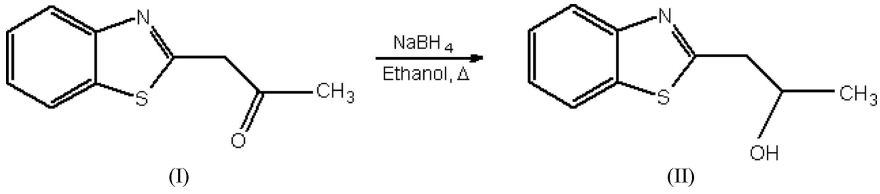
In the title compound, $C_{10}H_{11}NOS$, the asymmetric unit contains two molecules. The structure is stabilized by an intermolecular O—H···N hydrogen bond.

Comment

Heterocycles containing the thiazole moiety are present in many natural products which have useful biological activities (Carroll & Scheuer, 1990; Takita *et al.*, 1972). Benzothiazole derivatives have been shown to possess antitumoral (Bradshaw *et al.*, 2002), antimicrobial (Palmer *et al.*, 1971) and antioxidant (Ivanov & Yuritsyn, 1971) properties. The reduction of 1-(1,3-benzothiazol-2-yl)acetone, (I), using $NaBH_4$, selectively involves the C=O group to afford its alcohol, 1-(1,3-benzothiazol-2-yl)propan-2-ol, (II).



(I) (II)

The title molecule is shown in Fig. 1 and the selected geometric parameters are given in Table 1. All geometric parameters are in agreement with the corresponding ones for similar compounds (Saraçoğlu *et al.*, 2004; Büyükgüngör *et al.*, 2004; Aydın *et al.*, 2003, 2004; Allen *et al.*, 1987).

The benzothiazole groups are essentially planar, with maximum deviations of 0.016 (2) and 0.004 (2) Å for atoms C7

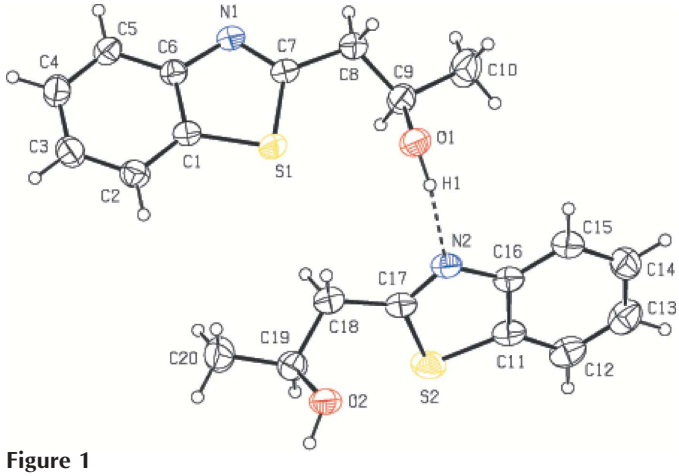


Figure 1
An *ORTEP-3* (Farrugia, 1997) drawing of the asymmetric unit of (II), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The intermolecular hydrogen bonding is indicated by a dashed line.

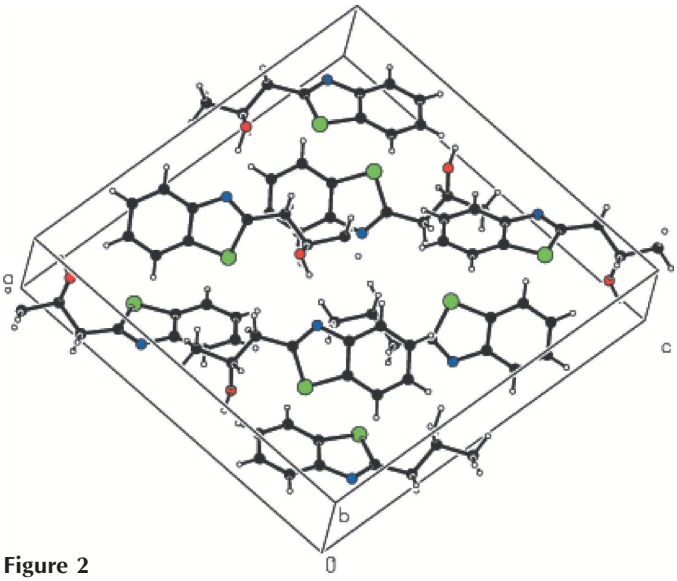


Figure 2
The packing diagram of (II).

and C16, respectively. The dihedral angle between the mean benzothiazole ring planes is 68.87 (8)°.

As can be seen from the packing diagram (Fig. 2), the molecules are elongated approximately parallel to the (101) plane and stacked along the *b* axis. The structure is stabilized by intermolecular O—H···N hydrogen bonding.

Experimental

$NaBH_4$ (0.4 g, 10.00 mmol) was added to a stirred solution of (I) (1.0 g, 5.25 mmol) in ethanol (50 ml). The reaction mixture was heated for 90 min at 313 K. The solvent was evaporated at reduced pressure and water (100 ml) was added. The mixture was extracted with dichloromethane (10 ml × 3). The organic layer was dried over Na_2SO_4 and evaporated in vacuum to obtain the pure product (II), which was recrystallized from ethanol (yield: 0.8 g, 80%; m.p. 371–373 K). IR (KBr; ν cm^{-1}): 3200–3400, 1509. ^{1}H NMR (300 MHz; $CDCl_3$): δ 1.34 (*d*, 3H, 6.3 Hz), 3.15–3.27 (*m*, 2H), 3.9 (*d*, 1H, 3 Hz), 4.32–4.43 (*m*, 1H), 7.34–7.98 (*m*, 4H arom). ^{13}C NMR (75 MHz, $CDCl_3$): δ 22.9 (CH_3), 42.6 (CH_2), 66.8 (CH), 121.6, 122.8, 125.1, 126.2, 134.8, 153.1, 169.3.

Crystal data

$C_{10}H_{11}NOS$
M_r = 193.27
Monoclinic, $P2_1/n$
a = 15.7702 (11) Å
b = 7.8856 (4) Å
c = 15.8703 (11) Å
β = 101.135 (5)°
V = 1936.4 (2) Å^3
Z = 8
D_x = 1.326 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2240 reflections
θ = 1.7–27.2°
μ = 0.29 mm^{-1}
T = 296 K
Prism, pale yellow
0.68 × 0.56 × 0.43 mm

Data collection

Stoe IPDS-II diffractometer
ω scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.826, T_{max} = 0.885
17123 measured reflections
4258 independent reflections
3250 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 27.1°
$h = -20 \rightarrow 20$
$k = -10 \rightarrow 10$
$l = -20 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118
S = 1.05
4258 reflections
245 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0653P)^2 + 0.2309P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.7297 (18)	O2—C19	1.422 (3)
S1—C7	1.7416 (18)	N1—C6	1.396 (2)
S2—C11	1.732 (2)	N1—C7	1.296 (2)
S2—C17	1.742 (2)	N2—C16	1.394 (2)
O1—C9	1.419 (3)	N2—C17	1.284 (3)
C1—S1—C7	89.38 (8)	O1—C9—C10	110.68 (18)
C11—S2—C17	89.78 (9)	O1—C9—C8	107.65 (17)
C6—N1—C7	111.05 (15)	S2—C11—C12	130.32 (16)
C16—N2—C17	111.48 (15)	S2—C11—C16	108.74 (13)
S1—C1—C6	109.56 (13)	N2—C16—C15	125.63 (16)
S1—C1—C2	129.50 (14)	N2—C16—C11	114.80 (16)
N1—C6—C5	125.50 (16)	S2—C17—C18	121.60 (15)
N1—C6—C1	114.45 (15)	N2—C17—C18	123.18 (18)
N1—C7—C8	122.48 (16)	S2—C17—N2	115.19 (14)
S1—C7—C8	121.98 (12)	O2—C19—C20	111.03 (19)
S1—C7—N1	115.54 (13)	O2—C19—C18	107.00 (17)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2	0.97 (3)	1.91 (3)	2.871 (2)	169 (3)

The O-bound H atoms were located in a difference map and refined freely [O—H = 0.89 (2)–0.97 (3) Å]. All other H atoms were positioned geometrically [0.93 and 0.98 (CH), 0.97 (CH_2) and 0.96 Å (CH_3)] and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 (1.5 for methyl) times U_{eq}(C).

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* for Windows (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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