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3-(1*H*-Benzimidazol-2-ylsulfanyl)propan-1-ol

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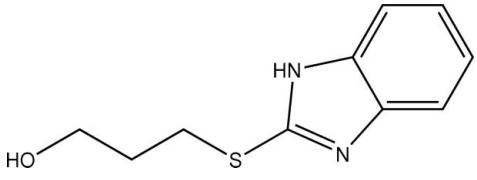
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.105; data-to-parameter ratio = 21.5.

Molecules of the title compound, $C_{10}H_{12}N_2OS$, are interconnected by N—H···O hydrogen bonds of moderate strength into infinite chains. There are also intramolecular O—H···N bonds of moderate length. Weaker interactions are represented by C—H···N bonds as well as by π–π interactions between the imidazole and benzene rings [distance between centroids = 3.6865 (8) Å].

Related literature

For related literature see: Dubey *et al.*, 1985; Garuti *et al.*, 2000. For the refinement weighting scheme, see: Prince (1982); Watkin (1994).



Experimental

Crystal data

$C_{10}H_{12}N_2OS$
M_r = 208.28
Monoclinic, $P2_1/c$
a = 7.1472 (3) Å
b = 11.5574 (6) Å
c = 12.5284 (6) Å
β = 98.343 (4)°
V = 1023.93 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 294 K
0.40 × 0.35 × 0.25 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
14014 measured reflections
2905 independent reflections
2469 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.105
S = 0.96
2897 reflections
135 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O14—H14···N2	0.84 (2)	1.93 (2)	2.746 (2)	163 (2)
N9—H9···O14^{i}	0.86 (2)	1.90 (2)	2.762 (2)	176 (2)
C11—H112···N2	0.98	2.47	2.978 (2)	112

Symmetry code: (i) $x-1, y, z$.

Data collection: *COLLECT* (Nonius, 1997); cell refinement: *DENZO/SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO/SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *CRYSTALS*.

We thank the Laboratoire de Physique des Interactions Ioniques and Spectropôle, Université de Provence, and Université Paul Cézanne, Faculté des Sciences et Techniques, Marseille, France, for the use of their Bruker–Nonius KappaCCD diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2063).

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supplementary materials

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3-(1*H*-Benzimidazol-2-ylsulfanyl)propan-1-ol

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Comment

Benzimidazole derivatives are important pharmaceutical intermediates. They are used in the design of antihelmintic (Dubey *et al.*, 1985) and antiviral pharmaceutics (Garuti *et al.*, 2000). Therefore we have decided to study this class of compounds. The title compound has been synthesized and its structure has been determined in order to study influence of new substituents on the biological activity of the new benzimidazole derivative.

In the title molecule the benzimidazole unit C1/N2/C3/C4/C5/C6/C7/C8/N9 is essentially planar, with a mean deviation of 0.0087 Å. The structure packing exhibits intra and intermolecular hydrogen bonds - see also Tab. 1 and Fig. 2.

Experimental

2 ml of triethylamine (19.98 mmol) and 3-chloropropan-1-ol (1.7 ml, 19.98 mmol) was added to 2-mercatobenzimidazole (1 g, 6.66 mmol) in dry ethanol (20 ml). The mixture was refluxed for 24 h. The solvent was evaporated in vacuum. The residue was purified by column chromatography on a silica gel (Elution: ethyl acetate/dichloromethane (1:9, *v*/*v*)) and the title compound was yielded as a yellow powder (1.12 g, 81%) with a melting point 395 K. The compound was dissolved in ethanol and pentane and after 72 h prismatic crystals were obtained. ^{1}H NMR(DMSO, 300 MHz) δ (p.p.m.):1.832–1.919 (m, 2H, CH_2S), 3.321–3.429 (m, 2H, CH2), 3.526 (m, 2H, CH_2O), 4.774 (s, 1H, OH), 7.078–7.440 (m, 4H, C_6H_4), 12.556 (s, 1H, NH). ^{13}C NMR (DMSO, 300 MHz) δ (p.p.m.):28.18 (CH_2S), 32.62 (CH_2), 59.09 (CH_2O), 110.60, 116.85, 121.38, 135.44, 143.42 (C4, C5, C6, C7, C8, C9), 150.50 (C═N).

Refinement

All the H atoms were discernable in a difference Fourier map. The C—H distances were contrained to 0.95 and 0.98 Å for aryl and methylene H atoms, respectively, while U_{iso}(H) = 1.2U_{eq}(C). The positional parameters as well as the U_{iso} of the H atoms H9 and H14, *i.e.* the H atoms involved in the N—H···O and O—H···N hydrogen bonds, respectively, were refined freely.

Figures

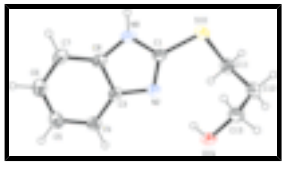

Fig. 1. A view of the title molecule with the atom labelling scheme. The displacement ellipsoids are drawn at the 30% probability level. The H atoms are shown as spheres of arbitary radius.

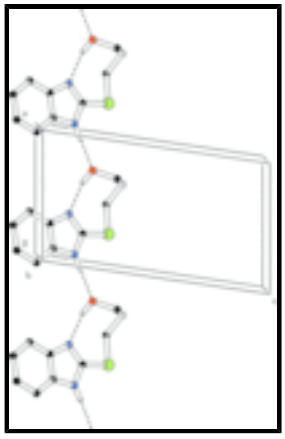

Fig. 2. A motif of the N—H···O hydrogen bonds forming the chains in the title structure.

3-(1*H*-Benzimidazol-2-ylsulfanyl)propan-1-ol

Crystal data

$C_{10}H_{12}N_2O_1S_1$	F_{000} = 440
M_r = 208.28	D_x = 1.351 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 395 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 7.1472 (3) Å	Cell parameters from 14014 reflections
b = 11.5574 (6) Å	θ = 2–30º
c = 12.5284 (6) Å	μ = 0.28 mm^{-1}
β = 98.343 (4)º	T = 294 K
V = 1023.93 (8) Å^3	Prism, yellow
Z = 4	0.40 × 0.35 × 0.25 mm

Data collection

Nonius KappaCCD diffractometer	2469 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.028
Monochromator: graphite	θ_{max} = 30.0º
T = 294 K	θ_{min} = 2.4º
φ scans	h = −10→10
Absorption correction: none	k = −16→16
14014 measured reflections	l = −17→17
2905 independent reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.039	H atoms treated by a mixture of independent and constrained refinement

	Method, part 1, Chebychev polynomial, (Watkin, 1994, *P*rince, 1982) [*w*eight] = 1.0/[A_0*T_0(x) + A_1*T_1(x) ··· + A_{n-1}]*T_{n-1}(x)]
$wR(F^2)$ = 0.105	where A_i are the Chebychev coefficients listed below and x = *F* /*F*max Method = Robust Weighting (*P*rince, 1982) W = [*w*eight] * [1-(delta*F*/6*sigma*F*)^2]^2 A_i are: 401. 643. 404. 180. 52.0
S = 0.96	$(\Delta/\sigma)_{max}$ = 0.001
2897 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
135 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
40 constraints	Extinction correction: None

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.20606 (16)	0.48268 (12)	0.70598 (10)	0.0398
N2	0.33956 (14)	0.46390 (10)	0.64550 (9)	0.0405
C3	0.25166 (16)	0.39740 (11)	0.55977 (10)	0.0367
C4	0.32332 (19)	0.35508 (12)	0.46994 (11)	0.0437
C5	0.2028 (2)	0.29163 (13)	0.39578 (11)	0.0500
C6	0.0160 (2)	0.27040 (13)	0.41022 (12)	0.0524
C7	−0.05715 (19)	0.31195 (12)	0.49875 (12)	0.0490
C8	0.06357 (16)	0.37607 (11)	0.57329 (10)	0.0382
N9	0.03898 (15)	0.43166 (10)	0.66774 (9)	0.0419
S10	0.22683 (5)	0.56461 (4)	0.82388 (3)	0.0543
C11	0.4478 (2)	0.64012 (12)	0.81673 (12)	0.0497
C12	0.6209 (2)	0.58824 (14)	0.88430 (12)	0.0519
C13	0.6655 (2)	0.46502 (14)	0.85854 (12)	0.0506
O14	0.70311 (14)	0.44920 (10)	0.75131 (9)	0.0511
H9	−0.063 (3)	0.4384 (16)	0.6965 (16)	0.061 (5)*
H14	0.602 (3)	0.4573 (17)	0.7080 (18)	0.067 (6)*
H7	−0.1845	0.2974	0.5083	0.0582*
H6	−0.0628	0.2262	0.3578	0.0621*
H5	0.2482	0.2619	0.3337	0.0604*
H4	0.4506	0.3693	0.4600	0.0533*
H111	0.4340	0.7200	0.8407	0.0592*
H112	0.4698	0.6400	0.7413	0.0592*
H121	0.6009	0.5917	0.9600	0.0613*
H122	0.7308	0.6355	0.8743	0.0613*
H131	0.7770	0.4400	0.9081	0.0607*
H132	0.5569	0.4168	0.8691	0.0607*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0318 (5)	0.0495 (7)	0.0390 (6)	0.0036 (5)	0.0086 (4)	0.0026 (5)
N2	0.0303 (4)	0.0541 (6)	0.0381 (5)	−0.0015 (4)	0.0078 (4)	−0.0024 (4)
C3	0.0320 (5)	0.0405 (6)	0.0378 (5)	0.0001 (4)	0.0061 (4)	0.0041 (4)

C4	0.0423 (6)	0.0493 (7)	0.0414 (6)	0.0001 (5)	0.0117 (5)	0.0020 (5)
C5	0.0627 (8)	0.0481 (7)	0.0401 (6)	−0.0025 (6)	0.0098 (6)	−0.0008 (5)
C6	0.0601 (8)	0.0460 (7)	0.0487 (7)	−0.0118 (6)	−0.0004 (6)	0.0013 (6)
C7	0.0394 (6)	0.0490 (7)	0.0569 (8)	−0.0090 (5)	0.0018 (5)	0.0076 (6)
C8	0.0331 (5)	0.0405 (6)	0.0413 (6)	0.0001 (4)	0.0068 (4)	0.0072 (5)
N9	0.0292 (5)	0.0530 (6)	0.0452 (6)	0.0016 (4)	0.0114 (4)	0.0040 (5)
S10	0.0455 (2)	0.0749 (3)	0.04444 (19)	0.00492 (16)	0.01321 (14)	−0.01196 (16)
C11	0.0562 (8)	0.0419 (6)	0.0508 (7)	0.0025 (6)	0.0069 (6)	−0.0057 (5)
C12	0.0499 (7)	0.0588 (8)	0.0460 (7)	−0.0021 (6)	0.0037 (6)	−0.0097 (6)
C13	0.0486 (7)	0.0607 (8)	0.0433 (7)	0.0115 (6)	0.0093 (5)	0.0015 (6)
O14	0.0320 (4)	0.0762 (7)	0.0464 (5)	0.0055 (4)	0.0097 (4)	−0.0085 (5)

Geometric parameters (Å, °)

C1—N2	1.3197 (15)	C8—N9	1.3800 (17)
C1—N9	1.3554 (16)	N9—H9	0.86 (2)
C1—S10	1.7427 (14)	S10—C11	1.8182 (16)
N2—C3	1.3939 (16)	C11—C12	1.517 (2)
C3—C4	1.3912 (17)	C11—H111	0.980
C3—C8	1.4009 (16)	C11—H112	0.980
C4—C5	1.382 (2)	C12—C13	1.505 (2)
C4—H4	0.950	C12—H121	0.980
C5—C6	1.395 (2)	C12—H122	0.980
C5—H5	0.950	C13—O14	1.4195 (17)
C6—C7	1.379 (2)	C13—H131	0.980
C6—H6	0.950	C13—H132	0.980
C7—C8	1.3899 (19)	O14—H14	0.84 (2)
C7—H7	0.950		
N2—C1—N9	113.50 (12)	C8—N9—H9	128.4 (13)
N2—C1—S10	126.61 (10)	C1—N9—H9	124.6 (13)
N9—C1—S10	119.89 (9)	C1—S10—C11	100.77 (6)
C1—N2—C3	104.51 (10)	S10—C11—C12	115.24 (11)
N2—C3—C4	129.75 (11)	S10—C11—H111	108.1
N2—C3—C8	109.70 (11)	C12—C11—H111	108.2
C4—C3—C8	120.55 (12)	S10—C11—H112	108.0
C3—C4—C5	117.63 (12)	C12—C11—H112	107.8
C3—C4—H4	121.2	H111—C11—H112	109.5
C5—C4—H4	121.2	C11—C12—C13	115.82 (12)
C4—C5—C6	121.39 (13)	C11—C12—H121	107.6
C4—C5—H5	119.3	C13—C12—H121	108.1
C6—C5—H5	119.3	C11—C12—H122	108.2
C5—C6—C7	121.64 (13)	C13—C12—H122	107.5
C5—C6—H6	119.2	H121—C12—H122	109.5
C7—C6—H6	119.2	C12—C13—O14	113.58 (13)
C6—C7—C8	117.08 (12)	C12—C13—H131	108.8
C6—C7—H7	121.5	O14—C13—H131	108.3
C8—C7—H7	121.5	C12—C13—H132	108.2
C3—C8—C7	121.71 (12)	O14—C13—H132	108.5
C3—C8—N9	105.40 (11)	H131—C13—H132	109.5

C7—C8—N9	132.88 (12)	C13—O14—H14	109.5 (14)
C8—N9—C1	106.88 (10)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O14—H14···N2	0.84 (2)	1.93 (2)	2.746 (2)	163 (2)
N9—H9···O14^{i}	0.86 (2)	1.90 (2)	2.762 (2)	176 (2)
C11—H112···N2	0.98	2.47	2.978 (2)	112

Symmetry codes: (i) *x*−1, *y*, *z*.

Fig. 1

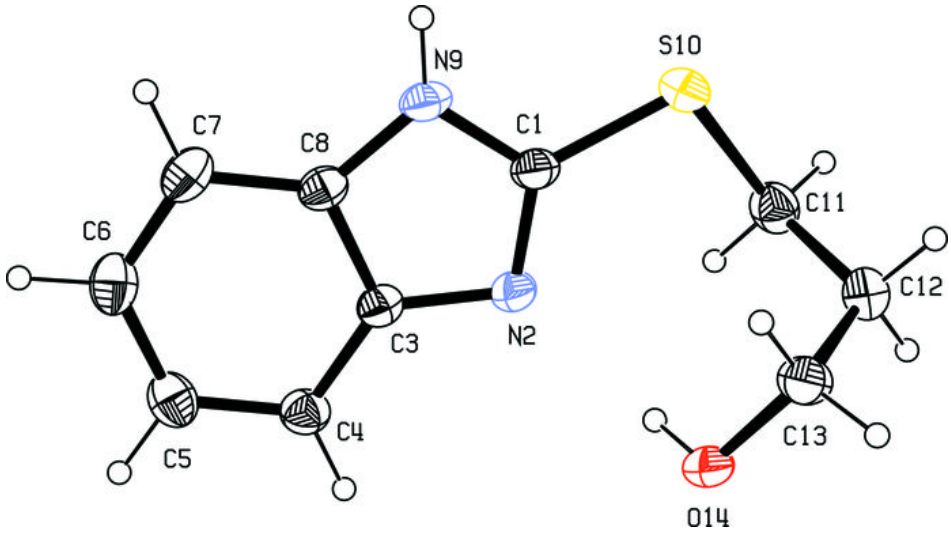

Fig. 2