Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Benzylsulfanyl-1*H*-benzimidazole

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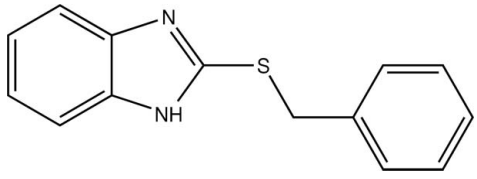
Received 25 October 2007; accepted 3 November 2007

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.003 Å; R factor = 0.038; wR factor = 0.069; data-to-parameter ratio = 14.2.

In the molecule of the title compound, $C_{14}H_{12}N_2S$, the benzimidazole ring system and the phenyl ring form a dihedral angle of 81.36 (7)°. The crystal structure exhibits intermolecular C—H···N and N—H···N hydrogen bonds.

Related literature

For related literature see: Carlsson *et al.* (2002); Easmon *et al.* (2001); Güneş & Coşar (1992); Küçükbay *et al.* (2004); Tebbe *et al.* (1997). For the refinement weighting scheme, see: Watkin (1994); Prince (1982).



Experimental

Crystal data

$C_{14}H_{12}N_2S$
M_r = 240.33
Monoclinic, $P2_1/c$
a = 12.373 (7) Å
b = 9.807 (5) Å
c = 9.942 (3) Å
β = 91.084 (3)°
V = 1206.2 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 294 K
0.40 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
8533 measured reflections
2236 independent reflections
1988 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.069
S = 0.93
2229 reflections
157 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 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
N7—H7···N2^{i}	0.87 (2)	2.05 (2)	2.915 (1)	173.50 (17)
C11—H111···N2^{i}	0.96	2.62	3.555 (3)	166

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

Data collection: *COLLECT* (Nonius, 2001); 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* (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 de Saint Jérôme, Avenue Escadrille Normandie Niemen, 13397 Marseille Cedex 20, France, for the use of their diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2161).

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supplementary materials

Acta Cryst. (2007). E**63**, o4551 [**doi:10.1107/S1600536807055687**]

2-Benzylsulfanyl-1*H*-benzimidazole

E. A. Yavo, R. Kakou-Yao, S. Coulibaly, A. Abou and A. J. Tenon

Comment

Benzimidazole derivatives are important pharmaceutical intermediates because of their therapeutic properties in modern drug discovery (Tebbe *et al.*, 1997). For example, omeprazole, which contains benzimidazole and pyridine, is the best selling anti-ulcer drug nowadays (Carlsson *et al.*, 2002). Benzimidazole derivatives generally exhibit versatile pharmacological activities, such as antibacterial, antifungal, antihelmintic, anti-allergic, antineoplastic, local analgesic, antihistaminic, vasodilative, hypotensive and spasmolytic activities (Easmon *et al.*, 2001; Güneş & Coşar, 1992; Küçükbay *et al.*, 2004). In order to have a better knowledge of their structure, we have embarked on a study of this class of compounds. The molecular structure of the title compound, $C_{14}H_{12}N_2S$ (I), and the atomic labeling scheme are shown in Fig.1. In this structure, the nine-membered benzimidazole ring system C1/N2/C3/C4/C5/C6/N7/C8/C9 is essentially planar, the maximum deviation from planarity being 0.022 (1) Å for atom N2. The phenyl ring C12/C13—C17 is connected to the benzimidazole ring system by the SCH_2 group. The classical intermolecular N—H···N hydrogen bond, which leads to the formation of infinite molecular chains along the [001] direction, and the weak C—H···N hydrogen bond consolidate the structure (Fig.2).

Experimental

Benzyl chloride (0.84 ml, 7.3 mmol) was added to 2-mercaptobenzimidazole (1 g, 6.7 mmol) in dry ethanol (15 ml). The mixture was refluxed for 7 h. The reaction mixture was diluted with ethyl acetate, and the resulting solid was collected and dissolved in 15 ml of water. 30 ml of a solution of sodium hydrogen carbonate (30 g in 100 ml of water) was then added. A white powder was isolated by filtration and dried to give (I) as colorless crystals (1.4 g, 88%), mp: 397 K. ^{1}H NMR (CD_3COCD_3, 300 MHz, p.pm.) δ: 4.09 (s, 2H, CH_2); 7.19–7.35 (2 m, 9H, H aromatic); 12.5 (1*H*, NH). ^{13}C NMR (CD_3COCD_3, 300 MHz, p.pm.) δ: 34.3 (CH2); 116.5–127.9 (C_6H_5 and C_6H_4); 168.3 (C═N).

Refinement

The H atom bonded to N7 was located in a difference Fourier map; the positional parameters and U_{iso} were refined freely. Other H atoms were placed at calculated positions, with C—H = 0.93 Å (aromatic) or 0.96 Å (methylene) and refined using a riding model with U_{iso}(H) constrained to be 1.2U_{eq}(C).

Figures

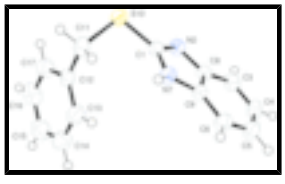

Fig. 1. The molecular structure of (I) showing the atomic labeling scheme, with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radius.

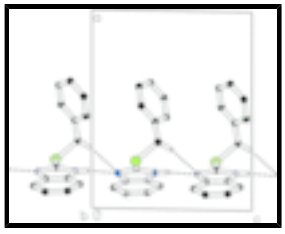

Fig. 2. Crystal packing of compound (I) viewed down the *b* axis, showing the hydrogen bond C—H···N and the hydrogen-bonded chains N—H···N along the *c* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonds have been omitted for clarity.

2-Benzylsulfanyl-1*H*-benzimidazole

Crystal data

$C_{14}H_{12}N_2S_1$	F_{000} = 504
M_r = 240.33	D_x = 1.323 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 397 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.373 (7) Å	Cell parameters from 8533 reflections
b = 9.807 (5) Å	θ = 1.7–26.1º
c = 9.942 (3) Å	μ = 0.25 mm^{-1}
β = 91.084 (3)º	T = 294 K
V = 1206.2 (10) Å^3	Block, colorless
Z = 4	0.40 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD diffractometer	1988 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.035
Monochromator: graphite	θ_{max} = 26.1º
T = 294 K	θ_{min} = 1.7º
φ scans	h = −15→15
Absorption correction: none	k = −12→12
8533 measured reflections	l = −11→11
2236 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.038	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.069	$w = [1-(F_o-F_c)^2/36\sigma^2(F)]^2/[168T_0(x) + 239T_1(x) + 121T_2(x) + 25.6T_3(x)]$ where T_i are Chebychev polynomials and x = F_c/F_{max} (*P*rince, 1982; Watkin, 1994)
S = 0.93	$(\Delta/\sigma)_{max}$ = 0.0002

2229 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
157 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
44 constraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Refinement. The reflections 1 0 0; 2 0 0; 1 1 0; 2 1 0;-1 1 1; 0 1 1; 1 1 1 have been measured with too low intensities. It might be caused by some systematical error, probably by shielding by a beam stop of these diffractions. They were not used in the refinement.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
H3	0.8977	0.5371	0.9572	0.0468*
H4	0.9477	0.7303	0.8390	0.0562*
H5	0.9362	0.7373	0.6089	0.0552*
H6	0.8783	0.5489	0.4847	0.0480*
H7	0.8127 (14)	0.2722 (19)	0.528 (2)	0.048 (5)*
H13	0.5879	0.2781	0.4779	0.0600*
H14	0.4254	0.3911	0.5037	0.0756*
H15	0.2973	0.3051	0.6440	0.0744*
H16	0.3322	0.1087	0.7641	0.0696*
H17	0.4954	−0.0036	0.7410	0.0564*
C1	0.79925 (12)	0.23145 (15)	0.72299 (15)	0.0308
N2	0.82205 (10)	0.29955 (13)	0.83423 (13)	0.0320
C3	0.89447 (13)	0.53917 (17)	0.86371 (17)	0.0393
C4	0.92308 (14)	0.65360 (18)	0.79260 (19)	0.0460
C5	0.91706 (14)	0.65750 (18)	0.65297 (19)	0.0462
C6	0.88252 (13)	0.54683 (17)	0.57815 (18)	0.0397
N7	0.81656 (11)	0.30395 (13)	0.60891 (13)	0.0324
C8	0.85906 (11)	0.42602 (15)	0.78982 (15)	0.0299
C9	0.85465 (11)	0.43068 (15)	0.64996 (15)	0.0293
S10	0.75958 (4)	0.06141 (4)	0.72740 (5)	0.0435
C11	0.66222 (13)	0.04929 (18)	0.58752 (18)	0.0412
C12	0.55881 (13)	0.12579 (16)	0.60721 (17)	0.0370
C13	0.53667 (16)	0.24409 (19)	0.5364 (2)	0.0504
C14	0.43910 (19)	0.3110 (2)	0.5511 (2)	0.0628
C15	0.36300 (18)	0.2602 (2)	0.6351 (2)	0.0618
C16	0.38381 (16)	0.1429 (2)	0.7063 (2)	0.0583
C17	0.48110 (15)	0.0758 (2)	0.69275 (19)	0.0475
H111	0.6957	0.0843	0.5083	0.0492*
H112	0.6449	−0.0453	0.5745	0.0492*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0341 (8)	0.0334 (8)	0.0248 (8)	0.0003 (6)	−0.0003 (6)	0.0008 (6)

N2	0.0372 (7)	0.0359 (7)	0.0229 (7)	−0.0006 (5)	0.0000 (5)	−0.0001 (5)
C3	0.0426 (9)	0.0458 (10)	0.0293 (9)	−0.0035 (7)	−0.0026 (7)	−0.0077 (7)
C4	0.0458 (10)	0.0411 (9)	0.0511 (12)	−0.0106 (8)	−0.0007 (8)	−0.0103 (8)
C5	0.0509 (10)	0.0391 (9)	0.0488 (12)	−0.0115 (8)	0.0031 (8)	0.0049 (8)
C6	0.0467 (9)	0.0434 (9)	0.0292 (9)	−0.0037 (7)	0.0037 (7)	0.0052 (7)
N7	0.0419 (7)	0.0353 (7)	0.0199 (7)	−0.0033 (6)	0.0009 (5)	−0.0033 (5)
C8	0.0307 (7)	0.0349 (8)	0.0241 (8)	0.0005 (6)	0.0005 (6)	−0.0016 (6)
C9	0.0297 (7)	0.0328 (8)	0.0256 (8)	−0.0003 (6)	0.0022 (6)	−0.0023 (6)
S10	0.0553 (3)	0.0336 (2)	0.0411 (3)	−0.00599 (19)	−0.00933 (19)	0.00478 (17)
C11	0.0471 (9)	0.0412 (9)	0.0354 (10)	−0.0087 (7)	−0.0012 (7)	−0.0084 (7)
C12	0.0448 (9)	0.0369 (9)	0.0291 (9)	−0.0079 (7)	−0.0029 (7)	−0.0058 (6)
C13	0.0613 (12)	0.0435 (10)	0.0462 (12)	−0.0089 (9)	−0.0016 (9)	0.0029 (8)
C14	0.0740 (14)	0.0419 (11)	0.0716 (16)	0.0053 (10)	−0.0178 (12)	−0.0045 (10)
C15	0.0572 (12)	0.0585 (13)	0.0692 (16)	0.0094 (10)	−0.0123 (11)	−0.0262 (11)
C16	0.0469 (11)	0.0806 (15)	0.0476 (13)	−0.0095 (10)	0.0048 (9)	−0.0138 (10)
C17	0.0496 (10)	0.0544 (11)	0.0383 (11)	−0.0070 (8)	−0.0014 (8)	0.0034 (8)

Geometric parameters (Å, °)

H3—C3	0.930	C4—C5	1.389 (3)
H4—C4	0.930	C5—C6	1.379 (2)
H5—C5	0.930	C6—C9	1.391 (2)
H6—C6	0.930	N7—C9	1.388 (2)
H7—N7	0.87 (2)	C8—C9	1.391 (2)
H13—C13	0.930	S10—C11	1.8264 (18)
H14—C14	0.930	C11—C12	1.499 (2)
H15—C15	0.930	C11—H111	0.960
H16—C16	0.930	C11—H112	0.960
H17—C17	0.930	C12—C13	1.382 (2)
C1—N2	1.3179 (19)	C12—C17	1.385 (2)
C1—N7	1.359 (2)	C13—C14	1.384 (3)
C1—S10	1.7391 (17)	C14—C15	1.365 (3)
N2—C8	1.397 (2)	C15—C16	1.372 (3)
C3—C4	1.376 (3)	C16—C17	1.381 (3)
C3—C8	1.397 (2)		
N2—C1—N7	113.62 (14)	C1—S10—C11	103.04 (8)
N2—C1—S10	121.39 (12)	S10—C11—C12	114.85 (12)
N7—C1—S10	124.86 (12)	S10—C11—H111	108.2
C1—N2—C8	104.54 (13)	C12—C11—H111	108.1
H3—C3—C4	121.6	S10—C11—H112	107.9
H3—C3—C8	121.0	C12—C11—H112	108.2
C4—C3—C8	117.32 (17)	H111—C11—H112	109.5
H4—C4—C3	119.3	C11—C12—C13	121.00 (16)
H4—C4—C5	118.9	C11—C12—C17	120.48 (16)
C3—C4—C5	121.75 (16)	C13—C12—C17	118.46 (17)
C4—C5—H5	119.0	C12—C13—H13	119.2
C4—C5—C6	121.84 (16)	C12—C13—C14	120.60 (19)
H5—C5—C6	119.2	H13—C13—C14	120.2
H6—C6—C5	122.2	C13—C14—H14	119.9

H6—C6—C9	121.4	C13—C14—C15	120.3 (2)
C5—C6—C9	116.41 (17)	H14—C14—C15	119.8
C1—N7—H7	125.7 (13)	H15—C15—C14	120.0
C1—N7—C9	106.32 (13)	H15—C15—C16	120.3
H7—N7—C9	127.5 (13)	C14—C15—C16	119.8 (2)
N2—C8—C3	129.85 (15)	H16—C16—C15	119.8
N2—C8—C9	109.77 (13)	H16—C16—C17	119.9
C3—C8—C9	120.37 (15)	C15—C16—C17	120.3 (2)
C8—C9—C6	122.30 (15)	C12—C17—C16	120.51 (19)
C8—C9—N7	105.74 (13)	C12—C17—H17	119.0
C6—C9—N7	131.94 (15)	C16—C17—H17	120.4

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N7—H7···N2^{i}	0.87 (2)	2.05 (2)	2.915 (1)	173.50 (17)
C11—H111···N2^{i}	0.96	2.62	3.555 (3)	166

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2.

Fig. 1

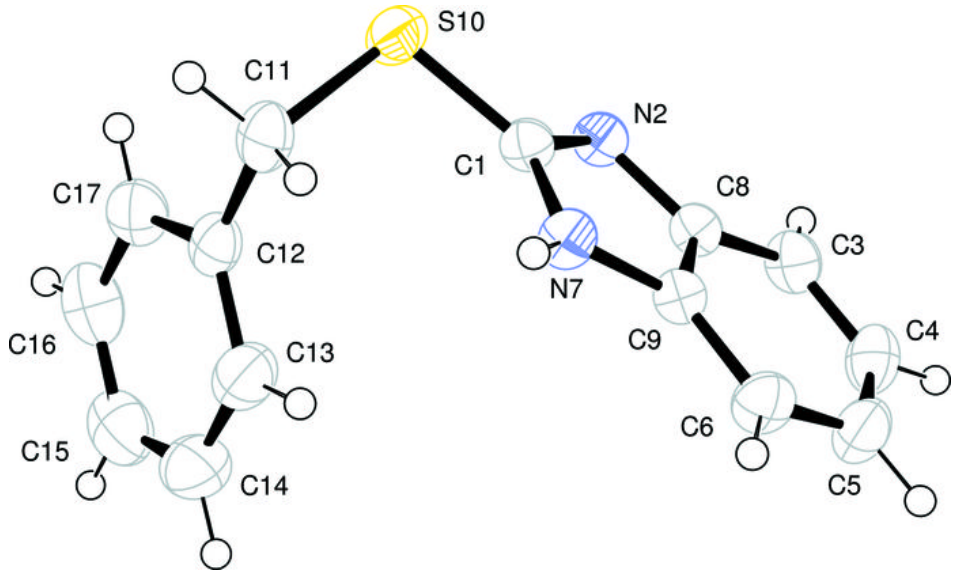

Fig. 2