Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Bromophenyl)thiazolo[3,2-*a*]-benzimidazole

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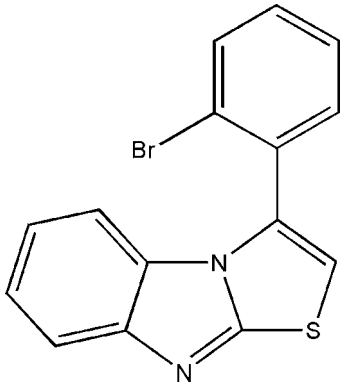
Received 17 August 2011; accepted 25 August 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.006 Å; R factor = 0.047; wR factor = 0.120; data-to-parameter ratio = 14.6.

The title compound, $C_{15}H_9BrN_2S$, was prepared by the reaction of 1-bromo-2-(2,2-dibromovinyl)benzene with 1*H*-benzo[*d*]imidazole-2(3*H*)-thione. The thiazolo[3,2-*a*]benzimidazole fused-ring system is nearly planar, the maximum atomic deviation being 0.049 (4) Å. This mean plane is oriented at a dihedral angle of 71.55 (17)° with respect ot the bromophenyl ring. π–π stacking is observed in the crystal structure, the centroid–centroid distance between the thiazole and imidazole rings of adjacent molecules being 3.582 (2) Å.

Related literature

For the biological activity of imidazoles and their use as inhibitors of neurodegenerative disorders and as antitumor drugs, see: Park *et al.* (1977); Schuckmann *et al.* (1979). For related imidazole compounds, see: Andreani *et al.* (2005); Xu *et al.* (2010).



Experimental

Crystal data

$C_{15}H_9BrN_2S$
M_r = 329.21
Monoclinic, $P2_1/c$
a = 11.2459 (19) Å
b = 9.1554 (16) Å
c = 14.2842 (18) Å
β = 118.159 (9)°
V = 1296.6 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.32 mm^{-1}
T = 296 K
0.24 × 0.22 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.456, T_{max} = 0.483
7492 measured reflections
2533 independent reflections
1977 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.120
S = 1.01
2533 reflections
173 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −1.20 e Å^{-3}

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported financially by the Priority Academic Development Program of Jiangsu Higher Education Institutions, China.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5299).

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supporting information

Acta Cryst. (2011). E**67**, o2540 [doi:10.1107/S1600536811034842]

3-(2-Bromophenyl)thiazolo[3,2-*a*]benzimidazole

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S1. Comment

Owing to the promising biological activities as inhibitors of neurodegenerative disorders and antitumor drugs, such compound structures have been studied (Park *et al.*, 1977; Schuckmann *et al.*, 1979). In the past decades, most of these investigations were carried out with imidazole (Andreani *et al.*, 2005; Xu *et al.*, 2010). We herein present the structure of 3-(2-bromopheny)thiazolo[3,2-*a*]benzimidazole(Fig. 1).

In the title compound, the benzene imidazole ring and thiazole ring are almost in the same plane. In the crystal structure, π-π interactions contribute the crystal packing.

S2. Experimental

1-Bromo-2-(2,2-dibromovinyl)benzene(1.2 mmol) in 1.0 ml of DMF were added to a stirred solution of 1*H*-benzo[*d*]imidazole-2(3*H*)-thione(1.0 mmol), Cs_2CO_3(2 mmol), CuI(0.1 mmol) and dmeda(0.2 mmol) in DMF(3 ml) under nitrogen. The resulting mixture was stirred at 100 °C for 4 h. After being cooled to room temperature, the reaction mixture was diluted with water and extracted with $CHCl_3$, the combined organic layer were dried over Na_2SO_4 and concentrated. The crude product was further purified by flash column chromatography using petroleum ether (PE) and CH_2Cl_2 as a white solid (90% yield). Single crystals suitable for X-ray diffraction were obtained by evaporation of an ethanol solution.

S3. Refinement

All the H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 Å, and with U_{iso}(H)= 1.2 U_{eq}(C).

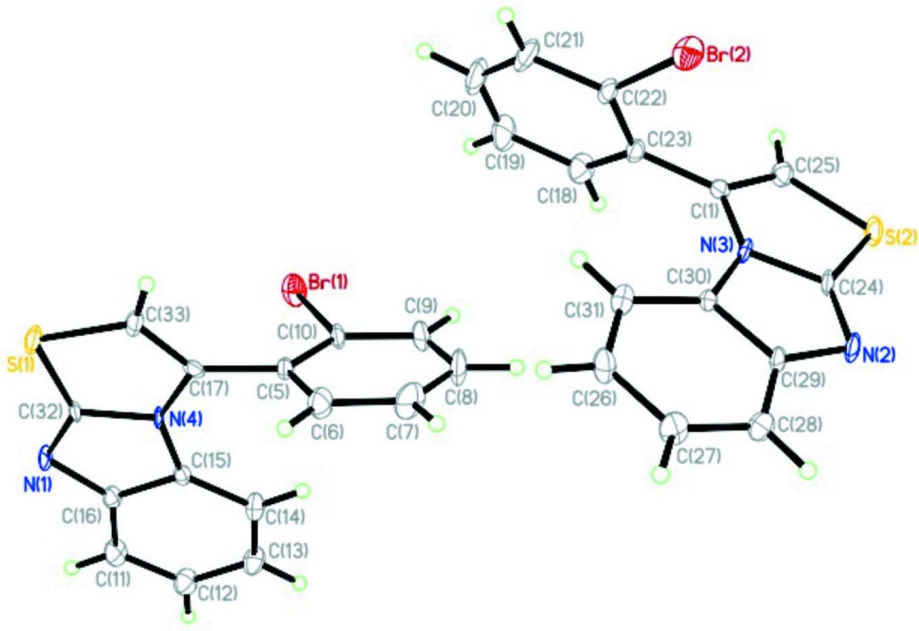

Figure 1

The molecular structure.

3-(2-Bromophenyl)thiazolo[3,2-*a*]benzimidazole

Crystal data

$C_{15}H_9BrN_2S$
$M_r = 329.21$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.2459\ (19)$ Å
$b = 9.1554\ (16)$ Å
$c = 14.2842\ (18)$ Å
$\beta = 118.159\ (9)°$
$V = 1296.6\ (4)$ Å^3
$Z = 4$

$F(000) = 656$
$D_x = 1.686$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3173 reflections
$\theta = 2.8–27.3°$
$\mu = 3.32$ mm^{-1}
$T = 296$ K
Block, colourless
0.24 × 0.22 × 0.22 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{min} = 0.456$, $T_{max} = 0.483$

7492 measured reflections
2533 independent reflections
1977 reflections with $I > 2\sigma(I)$
$R_{int} = 0.073$
$\theta_{max} = 26.0°$, $\theta_{min} = 2.1°$
$h = -13\rightarrow11$
$k = -11\rightarrow10$
$l = -11\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.120$
$S = 1.01$

2533 reflections
173 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0717P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -1.20$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.198 (7)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.22834 (4)	0.45478 (5)	0.55293 (3)	0.0445 (2)
C1	0.2162 (3)	0.0447 (4)	0.5360 (3)	0.0337 (9)
H1	0.1460	0.0949	0.4811	0.040*
C2	0.1918 (4)	−0.0647 (4)	0.5901 (3)	0.0414 (10)
H2	0.1033	−0.0901	0.5711	0.050*
C3	0.2968 (4)	−0.1382 (4)	0.6728 (3)	0.0407 (9)
H3	0.2766	−0.2115	0.7082	0.049*
C4	0.4298 (4)	−0.1059 (4)	0.7041 (3)	0.0389 (9)
H4	0.4991	−0.1562	0.7596	0.047*
C5	0.4574 (3)	0.0052 (4)	0.6498 (3)	0.0295 (8)
C6	0.3489 (3)	0.0771 (3)	0.5661 (3)	0.0239 (7)
C7	0.5470 (3)	0.1543 (4)	0.5890 (3)	0.0271 (7)
C8	0.4831 (3)	0.3354 (4)	0.4467 (3)	0.0315 (8)
H8	0.4781	0.4050	0.3975	0.038*
C9	0.3737 (3)	0.2780 (4)	0.4475 (3)	0.0258 (7)
C10	0.2316 (3)	0.3134 (4)	0.3760 (3)	0.0282 (7)
C11	0.1737 (4)	0.2726 (5)	0.2701 (3)	0.0429 (9)
H11	0.2244	0.2219	0.2449	0.052*
C12	0.0396 (5)	0.3077 (5)	0.2014 (4)	0.0592 (13)
H12	0.0014	0.2812	0.1302	0.071*
C13	−0.0352 (4)	0.3798 (6)	0.2377 (4)	0.0589 (13)
H13	−0.1247	0.4020	0.1912	0.071*
C14	0.0187 (4)	0.4208 (5)	0.3418 (4)	0.0474 (11)
H14	−0.0338	0.4697	0.3662	0.057*
C15	0.1524 (3)	0.3888 (4)	0.4105 (3)	0.0297 (8)
N1	0.4104 (2)	0.1755 (3)	0.5283 (2)	0.0250 (6)
N2	0.5811 (3)	0.0540 (3)	0.6619 (2)	0.0322 (7)
S1	0.63442 (8)	0.26789 (10)	0.54574 (8)	0.0354 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0387 (3)	0.0568 (3)	0.0447 (3)	0.00761 (17)	0.0251 (2)	−0.00393 (19)
C1	0.0233 (18)	0.041 (2)	0.031 (2)	0.0051 (15)	0.0084 (16)	0.0037 (16)
C2	0.031 (2)	0.053 (2)	0.043 (2)	−0.0045 (18)	0.0195 (19)	0.0010 (19)
C3	0.039 (2)	0.047 (2)	0.029 (2)	−0.0060 (18)	0.0110 (18)	0.0045 (18)
C4	0.038 (2)	0.042 (2)	0.0250 (19)	0.0043 (18)	0.0055 (17)	0.0051 (17)
C5	0.0222 (17)	0.0344 (17)	0.0216 (17)	0.0006 (15)	0.0019 (15)	−0.0037 (15)
C6	0.0208 (16)	0.0267 (16)	0.0207 (16)	0.0022 (13)	0.0068 (14)	−0.0020 (13)
C7	0.0158 (15)	0.0326 (17)	0.0258 (18)	0.0004 (14)	0.0040 (14)	−0.0081 (15)
C8	0.0235 (17)	0.0360 (19)	0.034 (2)	−0.0002 (15)	0.0129 (16)	−0.0026 (16)
C9	0.0224 (16)	0.0286 (17)	0.0263 (17)	0.0033 (13)	0.0114 (15)	−0.0006 (14)
C10	0.0226 (16)	0.0301 (17)	0.0272 (18)	0.0010 (14)	0.0078 (15)	0.0053 (15)
C11	0.040 (2)	0.049 (2)	0.031 (2)	0.0004 (18)	0.0089 (19)	−0.0024 (18)
C12	0.043 (3)	0.068 (3)	0.035 (2)	−0.001 (2)	−0.008 (2)	0.004 (2)
C13	0.025 (2)	0.067 (3)	0.057 (3)	0.002 (2)	−0.003 (2)	0.012 (3)
C14	0.025 (2)	0.051 (2)	0.063 (3)	0.0114 (18)	0.018 (2)	0.014 (2)
C15	0.0177 (16)	0.0358 (19)	0.0328 (19)	0.0018 (14)	0.0098 (15)	0.0038 (15)
N1	0.0135 (13)	0.0307 (14)	0.0253 (15)	0.0040 (11)	0.0046 (12)	−0.0023 (12)
N2	0.0181 (14)	0.0375 (16)	0.0261 (16)	0.0029 (12)	−0.0017 (13)	−0.0020 (14)
S1	0.0167 (4)	0.0451 (6)	0.0409 (6)	−0.0022 (4)	0.0107 (4)	−0.0042 (4)

Geometric parameters (Å, º)

Br1—C15	1.895 (4)	C8—C9	1.343 (5)
C1—C2	1.370 (5)	C8—S1	1.735 (4)
C1—C6	1.377 (5)	C8—H8	0.9300
C1—H1	0.9300	C9—N1	1.390 (4)
C2—C3	1.388 (6)	C9—C10	1.470 (5)
C2—H2	0.9300	C10—C11	1.386 (5)
C3—C4	1.376 (6)	C10—C15	1.388 (5)
C3—H3	0.9300	C11—C12	1.395 (6)
C4—C5	1.400 (6)	C11—H11	0.9300
C4—H4	0.9300	C12—C13	1.351 (7)
C5—N2	1.392 (5)	C12—H12	0.9300
C5—C6	1.405 (5)	C13—C14	1.367 (7)
C6—N1	1.391 (4)	C13—H13	0.9300
C7—N2	1.304 (5)	C14—C15	1.385 (5)
C7—N1	1.375 (4)	C14—H14	0.9300
C7—S1	1.732 (4)		
C2—C1—C6	117.2 (3)	C8—C9—C10	127.4 (3)
C2—C1—H1	121.4	N1—C9—C10	121.7 (3)
C6—C1—H1	121.4	C11—C10—C15	118.2 (3)
C1—C2—C3	121.3 (4)	C11—C10—C9	119.6 (3)
C1—C2—H2	119.4	C15—C10—C9	122.2 (3)
C3—C2—H2	119.4	C10—C11—C12	120.0 (4)

C4—C3—C2	122.0 (4)	C10—C11—H11	120.0
C4—C3—H3	119.0	C12—C11—H11	120.0
C2—C3—H3	119.0	C13—C12—C11	120.3 (4)
C3—C4—C5	117.9 (3)	C13—C12—H12	119.8
C3—C4—H4	121.1	C11—C12—H12	119.8
C5—C4—H4	121.1	C12—C13—C14	121.0 (4)
N2—C5—C4	129.4 (3)	C12—C13—H13	119.5
N2—C5—C6	111.7 (3)	C14—C13—H13	119.5
C4—C5—C6	118.8 (3)	C13—C14—C15	119.3 (4)
C1—C6—N1	133.0 (3)	C13—C14—H14	120.4
C1—C6—C5	122.9 (3)	C15—C14—H14	120.4
N1—C6—C5	104.1 (3)	C14—C15—C10	121.2 (4)
N2—C7—N1	115.0 (3)	C14—C15—Br1	118.8 (3)
N2—C7—S1	134.9 (3)	C10—C15—Br1	120.0 (2)
N1—C7—S1	110.1 (3)	C7—N1—C9	115.1 (3)
C9—C8—S1	113.8 (3)	C7—N1—C6	106.0 (3)
C9—C8—H8	123.1	C9—N1—C6	138.8 (3)
S1—C8—H8	123.1	C7—N2—C5	103.1 (3)
C8—C9—N1	110.9 (3)	C7—S1—C8	90.07 (16)