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3-Benzyl-5-benzylidene-2-sulfanylidene-1,3-thiazolidin-4-one

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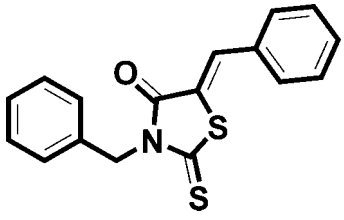
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.101; data-to-parameter ratio = 18.9.

In the title molecule, $C_{17}H_{13}NOS_2$, the essentially planar thiazole ring (r.m.s deviation 0.005 Å) forms dihedral angles of 16.85 (8)° and 75.02 (8)° with the phenyl rings. The dihedral angle between the two phenyl rings is 61.95 (9)°.

Related literature

For the synthesis and related structures, see: Shahwar *et al.* (2009, 2011).



Experimental

Crystal data

$C_{17}H_{13}NOS_2$
M_r = 311.40
Triclinic, $P\overline{1}$
a = 6.3152 (2) Å
b = 10.8168 (3) Å
c = 11.4545 (3) Å
α = 84.1150 (9)°
β = 77.6000 (9)°
γ = 76.1770 (9)°
V = 740.99 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 296 K
0.35 × 0.31 × 0.15 mm

Data collection

Bruker Kappa APEX II CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.886, T_{max} = 0.949
13205 measured reflections
3583 independent reflections
2930 reflections with $I > 2\sigma(I)$
R_{int} = 0.028

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.101
S = 1.03
3583 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH5281).

References

Bruker (2007). *SADABS*, *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Shahwar, D., Tahir, M. N., Raza, M. A., Ahmad, N. & Aslam, S. (2011). *Acta Cryst.* E**67**, o133.
Shahwar, D., Tahir, M. N., Raza, M. A. & Iqbal, B. (2009). *Acta Cryst.* E**65**, o2917.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supplementary materials

Acta Cryst. (2011). E**67**, o2083 [**doi:10.1107/S1600536811027450**]

3-Benzyl-5-benzylidene-2-sulfanylidene-1,3-thiazolidin-4-one

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Comment

The crystal structure determination of the title compound (I) is a countinuation of our work on thiazolidinone derivatives (Shahwar *et al.*, 2009, 2011).

The molecular structure of the title compound is shown in Fig. 1. The essentially planar thiazole ring [r.m.s deviation 0.005 Å] forms dihedral angles of 16.85 (8)° and 75.02 (8)° with the C5-C10 and C12-C17 phenyl rings, respectively. The dihedral angle between the two phenyl rings is 61.95 (9)°.

Experimental

The title compound was prepared following a previously published method (Shahwar *et al.*, 2009). X-ray quality crystals were grown from a solution of the title compound in n-hexane:ethylacetate:methanol (6:3:1).

Refinement

All H atoms were positioned with idealized geometry with C—H = 0.93 - 0.97 Å and were refined using a riding model with U_{iso}(H) = 1.2 U_{eq}(C). Four reflections 1 1 0, 0 0 1, 2 2 0 & 0 1 0 were omitted in the final refinemnt as they were obscured by the beamstop.

Figures

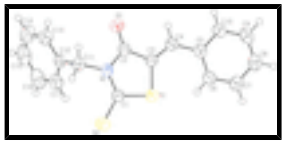


Fig. 1. The molecular structure of (I) with thermal ellipsoids drawn at the 50% probability level.

3-Benzyl-5-benzylidene-2-sulfanylidene-1,3-thiazolidin-4-one

Crystal data

$C_{17}H_{13}NOS_2$	$Z = 2$
$M_r = 311.40$	$F(000) = 324$
Triclinic, $P\overline{1}$	$D_x = 1.396$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 6.3152$ (2) Å	Cell parameters from 6403 reflections
$b = 10.8168$ (3) Å	$\theta = 2.6$–$28.3°$
$c = 11.4545$ (3) Å	$\mu = 0.36$ mm^{-1}
$\alpha = 84.1150$ (9)°	$T = 296$ K

β = 77.6000 (9)°	Needle, pale yellow
γ = 76.1770 (9)°	0.35 × 0.31 × 0.15 mm
V = 740.99 (4) Å^3	

Data collection

Bruker KAPPA APEX II CCD diffractometer	3583 independent reflections
Radiation source: fine-focus sealed tube	2930 reflections with $I > 2\sigma(I)$
graphite	R_{int} = 0.028
φ and ω scans	θ_{max} = 28.4°, θ_{min} = 3.4°
Absorption correction: multi-scan (*SADABS*;Bruker, 2007)	h = −8→8
T_{min} = 0.886, T_{max} = 0.949	k = −14→14
13205 measured reflections	l = −15→15

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.036	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.101	H-atom parameters constrained
S = 1.03	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.1921P]$ where $P = (F_o^2 + 2F_c^2)/3$
3583 reflections	$(\Delta/\sigma)_{max} < 0.001$
190 parameters	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
0 restraints	$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
S1	0.36101 (6)	0.34929 (4)	0.98088 (4)	0.04416 (12)
S2	0.24747 (8)	0.57799 (4)	0.82368 (4)	0.05631 (14)
O1	−0.0562 (2)	0.18668 (12)	0.89696 (10)	0.0518 (3)

N1	0.06938 (19)	0.37139 (12)	0.85045 (10)	0.0382 (3)
C3	0.2282 (2)	0.22259 (14)	0.99118 (13)	0.0374 (3)
C4	0.2515 (2)	0.11550 (14)	1.06168 (13)	0.0401 (3)
H4	0.1636	0.0602	1.0540	0.048*
C12	0.0019 (3)	0.36707 (14)	0.64596 (13)	0.0414 (3)
C5	0.3954 (2)	0.07342 (14)	1.14880 (13)	0.0401 (3)
C1	0.2109 (2)	0.43656 (15)	0.87728 (13)	0.0395 (3)
C2	0.0659 (2)	0.25206 (14)	0.91071 (12)	0.0384 (3)
C11	−0.0820 (2)	0.42216 (15)	0.76689 (13)	0.0430 (3)
H11A	−0.1013	0.5141	0.7575	0.052*
H11B	−0.2263	0.4036	0.8007	0.052*
C6	0.5720 (3)	0.12723 (16)	1.15454 (15)	0.0481 (4)
H6	0.6061	0.1920	1.0989	0.058*
C10	0.3525 (3)	−0.02573 (16)	1.23169 (16)	0.0529 (4)
H10	0.2383	−0.0650	1.2282	0.063*
C7	0.6974 (3)	0.08547 (18)	1.24193 (17)	0.0554 (4)
H7	0.8146	0.1226	1.2448	0.066*
C13	−0.1276 (3)	0.30505 (19)	0.60087 (17)	0.0594 (5)
H13	−0.2644	0.2959	0.6464	0.071*
C17	0.2039 (3)	0.38009 (18)	0.57709 (15)	0.0541 (4)
H17	0.2924	0.4226	0.6058	0.065*
C8	0.6501 (3)	−0.01051 (19)	1.32454 (18)	0.0611 (5)
H8	0.7336	−0.0378	1.3838	0.073*
C9	0.4783 (3)	−0.06585 (19)	1.31873 (19)	0.0651 (5)
H9	0.4466	−0.1312	1.3742	0.078*
C16	0.2752 (4)	0.3298 (2)	0.46494 (17)	0.0692 (6)
H16	0.4123	0.3378	0.4190	0.083*
C14	−0.0563 (5)	0.2564 (2)	0.4888 (2)	0.0784 (6)
H14	−0.1455	0.2152	0.4591	0.094*
C15	0.1443 (4)	0.2685 (2)	0.42184 (18)	0.0751 (7)
H15	0.1925	0.2351	0.3466	0.090*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0472 (2)	0.0448 (2)	0.0463 (2)	−0.01693 (16)	−0.01683 (16)	0.00314 (16)
S2	0.0700 (3)	0.0434 (2)	0.0624 (3)	−0.0228 (2)	−0.0220 (2)	0.00817 (19)
O1	0.0605 (7)	0.0539 (7)	0.0511 (7)	−0.0274 (5)	−0.0180 (5)	0.0010 (5)
N1	0.0415 (6)	0.0407 (7)	0.0344 (6)	−0.0112 (5)	−0.0093 (5)	−0.0016 (5)
C3	0.0404 (7)	0.0390 (7)	0.0334 (7)	−0.0110 (6)	−0.0054 (5)	−0.0041 (6)
C4	0.0456 (7)	0.0387 (7)	0.0369 (7)	−0.0114 (6)	−0.0061 (6)	−0.0053 (6)
C12	0.0501 (8)	0.0369 (7)	0.0364 (7)	−0.0052 (6)	−0.0152 (6)	0.0044 (6)
C5	0.0463 (7)	0.0344 (7)	0.0368 (7)	−0.0052 (6)	−0.0057 (6)	−0.0042 (6)
C1	0.0400 (7)	0.0418 (8)	0.0370 (7)	−0.0104 (6)	−0.0062 (6)	−0.0030 (6)
C2	0.0422 (7)	0.0427 (8)	0.0315 (7)	−0.0130 (6)	−0.0048 (5)	−0.0041 (6)
C11	0.0418 (7)	0.0464 (8)	0.0405 (8)	−0.0062 (6)	−0.0122 (6)	−0.0012 (6)
C6	0.0473 (8)	0.0483 (9)	0.0473 (9)	−0.0127 (7)	−0.0089 (7)	0.0082 (7)
C10	0.0631 (10)	0.0402 (8)	0.0598 (11)	−0.0171 (7)	−0.0197 (8)	0.0070 (7)

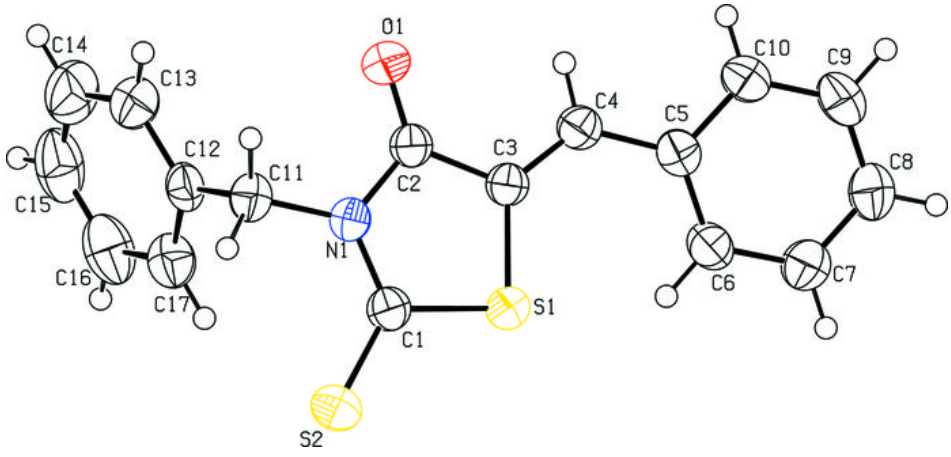
C7	0.0489 (9)	0.0575 (10)	0.0623 (11)	−0.0131 (7)	−0.0194 (8)	0.0050 (8)
C13	0.0733 (12)	0.0610 (11)	0.0518 (10)	−0.0236 (9)	−0.0208 (9)	−0.0012 (8)
C17	0.0549 (9)	0.0590 (11)	0.0459 (9)	−0.0099 (8)	−0.0092 (7)	0.0005 (8)
C8	0.0641 (11)	0.0582 (11)	0.0634 (11)	−0.0091 (8)	−0.0294 (9)	0.0113 (9)
C9	0.0786 (13)	0.0512 (10)	0.0684 (12)	−0.0191 (9)	−0.0279 (10)	0.0232 (9)
C16	0.0730 (12)	0.0707 (13)	0.0467 (10)	0.0048 (10)	−0.0005 (9)	0.0020 (9)
C14	0.1163 (19)	0.0720 (14)	0.0588 (13)	−0.0261 (13)	−0.0332 (13)	−0.0124 (10)
C15	0.1135 (19)	0.0592 (12)	0.0438 (10)	0.0038 (12)	−0.0195 (11)	−0.0085 (9)

Geometric parameters (Å, °)

S1—C1	1.7390 (15)	C6—C7	1.382 (2)
S1—C3	1.7517 (15)	C6—H6	0.9300
S2—C1	1.6389 (16)	C10—C9	1.379 (2)
O1—C2	1.2066 (18)	C10—H10	0.9300
N1—C1	1.3614 (19)	C7—C8	1.374 (3)
N1—C2	1.4026 (19)	C7—H7	0.9300
N1—C11	1.4715 (18)	C13—C14	1.380 (3)
C3—C4	1.339 (2)	C13—H13	0.9300
C3—C2	1.480 (2)	C17—C16	1.388 (3)
C4—C5	1.459 (2)	C17—H17	0.9300
C4—H4	0.9300	C8—C9	1.374 (3)
C12—C13	1.378 (2)	C8—H8	0.9300
C12—C17	1.379 (2)	C9—H9	0.9300
C12—C11	1.503 (2)	C16—C15	1.368 (3)
C5—C6	1.392 (2)	C16—H16	0.9300
C5—C10	1.395 (2)	C14—C15	1.361 (3)
C11—H11A	0.9700	C14—H14	0.9300
C11—H11B	0.9700	C15—H15	0.9300
C1—S1—C3	92.81 (7)	C7—C6—H6	119.6
C1—N1—C2	116.64 (12)	C5—C6—H6	119.6
C1—N1—C11	123.42 (13)	C9—C10—C5	120.40 (16)
C2—N1—C11	119.89 (12)	C9—C10—H10	119.8
C4—C3—C2	121.65 (13)	C5—C10—H10	119.8
C4—C3—S1	128.94 (12)	C8—C7—C6	120.44 (17)
C2—C3—S1	109.35 (10)	C8—C7—H7	119.8
C3—C4—C5	129.10 (14)	C6—C7—H7	119.8
C3—C4—H4	115.5	C12—C13—C14	120.65 (19)
C5—C4—H4	115.5	C12—C13—H13	119.7
C13—C12—C17	118.90 (16)	C14—C13—H13	119.7
C13—C12—C11	119.66 (15)	C12—C17—C16	120.04 (18)
C17—C12—C11	121.41 (15)	C12—C17—H17	120.0
C6—C5—C10	118.12 (14)	C16—C17—H17	120.0
C6—C5—C4	123.75 (14)	C7—C8—C9	119.40 (16)
C10—C5—C4	118.12 (14)	C7—C8—H8	120.3
N1—C1—S2	127.66 (12)	C9—C8—H8	120.3
N1—C1—S1	111.06 (11)	C8—C9—C10	120.86 (17)
S2—C1—S1	121.28 (9)	C8—C9—H9	119.6
O1—C2—N1	122.92 (13)	C10—C9—H9	119.6

O1—C2—C3	126.97 (14)	C15—C16—C17	120.2 (2)
N1—C2—C3	110.11 (12)	C15—C16—H16	119.9
N1—C11—C12	112.72 (12)	C17—C16—H16	119.9
N1—C11—H11A	109.0	C15—C14—C13	120.1 (2)
C12—C11—H11A	109.0	C15—C14—H14	119.9
N1—C11—H11B	109.0	C13—C14—H14	119.9
C12—C11—H11B	109.0	C14—C15—C16	120.13 (19)
H11A—C11—H11B	107.8	C14—C15—H15	119.9
C7—C6—C5	120.75 (15)	C16—C15—H15	119.9
C1—S1—C3—C4	−176.86 (14)	C1—N1—C11—C12	101.92 (16)
C1—S1—C3—C2	0.27 (11)	C2—N1—C11—C12	−80.68 (17)
C2—C3—C4—C5	−177.53 (14)	C13—C12—C11—N1	122.62 (16)
S1—C3—C4—C5	−0.7 (2)	C17—C12—C11—N1	−59.2 (2)
C3—C4—C5—C6	−14.8 (2)	C10—C5—C6—C7	−1.6 (2)
C3—C4—C5—C10	164.69 (16)	C4—C5—C6—C7	177.88 (15)
C2—N1—C1—S2	−178.75 (11)	C6—C5—C10—C9	1.9 (3)
C11—N1—C1—S2	−1.3 (2)	C4—C5—C10—C9	−177.57 (16)
C2—N1—C1—S1	1.48 (16)	C5—C6—C7—C8	0.3 (3)
C11—N1—C1—S1	178.95 (10)	C17—C12—C13—C14	0.2 (3)
C3—S1—C1—N1	−0.97 (11)	C11—C12—C13—C14	178.45 (17)
C3—S1—C1—S2	179.24 (10)	C13—C12—C17—C16	−0.8 (3)
C1—N1—C2—O1	178.07 (14)	C11—C12—C17—C16	−179.01 (15)
C11—N1—C2—O1	0.5 (2)	C6—C7—C8—C9	0.8 (3)
C1—N1—C2—C3	−1.27 (17)	C7—C8—C9—C10	−0.4 (3)
C11—N1—C2—C3	−178.83 (12)	C5—C10—C9—C8	−1.0 (3)
C4—C3—C2—O1	−1.5 (2)	C12—C17—C16—C15	0.8 (3)
S1—C3—C2—O1	−178.84 (13)	C12—C13—C14—C15	0.4 (3)
C4—C3—C2—N1	177.84 (13)	C13—C14—C15—C16	−0.5 (3)
S1—C3—C2—N1	0.46 (14)	C17—C16—C15—C14	−0.1 (3)

Fig. 1


O1
C14
C13
C12
C11
C2
C3
C4
C5
C10
C9
C8
C15
N1
C16
C17
C6
C7
S1
C1
S2