Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(*Z*)-3-Phenyl-2-(propan-2-ylidenehydrazono)-thiazolidin-4-one

Liang-Zhong Xu,[a]* Kai Li,[a] Hai-Bin Song,[b] Yong-Wei Huang[a] and Kai Zhou[a]

[a]College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China, and [b]State Key Laboratory and Institute of Elemento-Organic, Chemistry, Nankai University, Tianjin 300071, People's Republic of China

Correspondence e-mail: qknhs@163169.net

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.051
wR factor = 0.132
Data-to-parameter ratio = 13.5

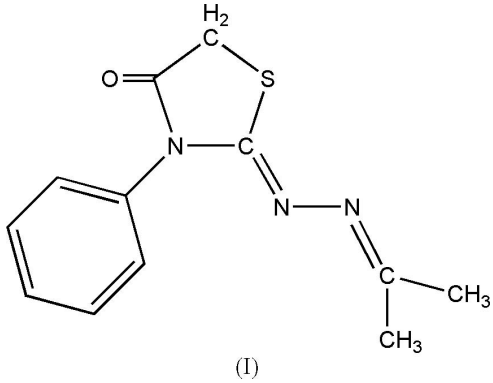
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 29 March 2005
Accepted 15 April 2005
Online 23 April 2005

In the title compound, $C_{12}H_{13}N_3OS$, the molecular backbone formed by the thiazolidinone and 2-(propan-2-ylidene)-hydrazone groups is planar. There are some weak intra- and intermolecular hydrogen-bond interactions which stabilize the crystal structure.

Comment

It has been reported that both thiazoles and thiazolidines have good and wide insecticidal, fungicidal, herbicidal and acaricidal activity (Melnikov, *et al.*, 1979; Kratt & Salberk, 1984). As part of our search for compounds with good herbicidal and fungicidal activity, the title compound, (I), was synthesized. We report here its crystal structure.



(I)

Bond lengths and angles in the thiazolidine ring (Table 1) are in agreement those reported previously (Buyuktimkin *et al.*, 1984; Yang *et al.*, 1995; Pomés Hernandez *et al.*, 1996). The molecular backbone formed by the thiazolidinone and 2-(propan-2-ylidene)hydrazone groups is essentially planar, the maximum deviations being −0.070 (3) and 0.029 (3)° for C2 and N2, respectively. The phenyl ring is twisted by 70.98 (7)° with respect to this plane. There are some weak C—H···O and C—H···N intra- and intermolecular hydrogen-bond interactions which stabilize the crystal structure (Table 2).

Experimental

A mixture of hydrazine (0.02 mol), ethyl chloroacetate (0.02 mol) and phenyl isothiocyanate (0.02 mol) was stirred in refluxing acetone (5 ml) for 5 h at 327 K to afford the title compound (3.71 g, yield 75%). Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Crystal data

$C_{12}H_{13}N_3OS$
$M_r = 247.31$
Monoclinic, $P2_1/c$
$a = 16.859\ (9)$ Å
$b = 5.667\ (3)$ Å
$c = 12.580\ (7)$ Å
$\beta = 90.685\ (9)^\circ$
$V = 1201.8\ (11)$ Å^3
$Z = 4$
$D_x = 1.367$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1528 reflections
$\theta = 2.4$–22.4°
$\mu = 0.26$ mm^{-1}
$T = 293\ (2)$ K
Block, yellow
$0.18 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.950$, $T_{max} = 0.970$
6139 measured reflections
2121 independent reflections
1093 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$
$\theta_{max} = 25.0^\circ$
$h = -20 \rightarrow 11$
$k = -6 \rightarrow 6$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.132$
$S = 0.89$
2121 reflections
157 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0657P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.010 (2)

Table 1
Selected geometric parameters (Å, °).

S1—C1	1.739 (3)	N2—C1	1.277 (4)
S1—C2	1.790 (3)	N2—N3	1.418 (4)
N1—C3	1.386 (4)	N3—C10	1.261 (4)
N1—C1	1.387 (4)		
C1—S1—C2	91.87 (15)	C1—N2—N3	107.7 (3)
C3—N1—C1	116.0 (3)	N2—C1—S1	125.3 (2)
C3—N1—C4	119.5 (2)	N1—C1—S1	112.2 (2)
C1—N1—C4	124.5 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···N2	0.96	2.30	2.739 (5)	107
C5—H5···O1^{i}	0.93	2.41	3.321 (4)	165
C8—H8···O1^{ii}	0.93	2.50	3.413 (4)	168

Symmetry codes: (i) $x, y-1, z$; (ii) $x, \frac{3}{2}-y, \frac{1}{2}+z$.

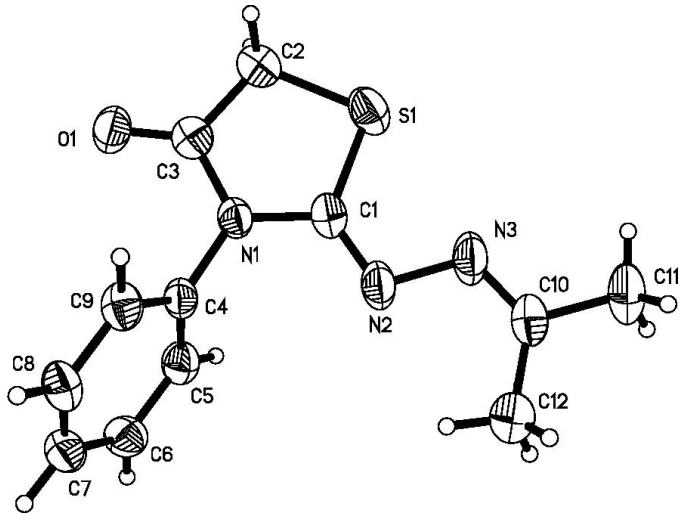


Figure 1
View of (I), with displacement ellipsoids drawn at the 40% probability level.

All H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$ for the aryl and methylene H atoms and $1.5U_{eq}(C)$ for the methyl H atoms.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

References

Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Buyuktimkin, S., Elz, S. & Schunack, W. (1984). *Arch. Pharm.* **317**, 787–802.
Kratt, G. & Salberk, G. (1984). Ger.n Patent DE 3505432.
Melnikov, N. N., Grapov, A. F., Razvodovskaya, G. K., Abelentseva, G. M., Sedykh, A. S., Shapovalova, G. K. & Siforova, T. A. (1979). Jpn Patent JP 78103471.
Pomés Hernández, R., Rodriguez, J. D., de Armas, H. N. & Toscano, R. A. (1996). *Acta Cryst.* C**52**, 1731–1733.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, D. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yang, H. Z., Liu, H. Y., Wu, Y., Wang, R. J. & Yao, X. K. (1995). *Chin. J. Struct. Chem.* **14**, 131–134.