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2-(1,3-Dithiolan-2-ylidene)-1-phenyl-2-(1,2,4-triazol-1-yl)ethanone

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.103
Data-to-parameter ratio = 15.4

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

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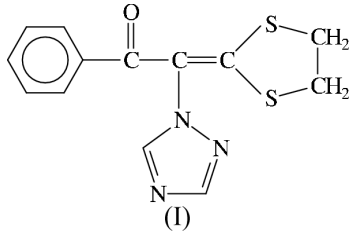
In the title compound, $C_{13}H_{11}N_3OS_2$, the dihedral angles between the planes of the triazole and phenyl rings and that through the four NC_3 atoms of the C=C are 76.(1) and 57.6 (1)°, respectively. There are some intermolecular interactions in the crystal structure.

Comment

Many *N*-heterocyclic compounds have been widely used as potent and broad-spectrum fungicides, such as buthilbate, fenarimol and nuarimol (Kato *et al.*, 1975; Gestel *et al.*, 1980). Compounds containing the triazole ring system are well known as efficient fungicides in agriculture and medicine, where they act by inhibiting the biosynthesis of ergosterol (Banting *et al.*, 1989). They have also good plant-growth regulatory activity on a wide variety of crops (Xu *et al.*, 2002). In order to search for new triazole compounds with higher bioactivity, the title compound, (I), was synthesized and its structure is reported here.



(I)

In compound (I), the bond lengths and angles are generally normal in the phenyl and triazole rings (Ji *et al.*, 2002). The C8—C9 bond length of 1.370 (4) Å is indicative of considerable double-bond character. The six atoms S1, S2, N3, C7, C8 and C9 lie in a plane (*P*1). The dihedral angles formed by the triazole ring with the phenyl ring (C1/C2/C3/C4/C5/C6) and *P*1 are 79.1 (1) and 76.5 (1)°, respectively. The dihedral angle between the phenyl ring and *P*1 is 57.6 (1)°. Torsion angles are given in Table 1.

The conformation of the dithiacyclopentane ring is half-chair, with a total puckering amplitude (Cremer & Pople, 1975) Q_T = 0.456 (3) Å and a pseudo-twofold axis running along the direction through C9 and the mid-point of the C10—C11 bond.

There are some weak intermolecular C—H···O and C—H···N hydrogen bonds (Table 2), which stabilize the structure of (I).

Experimental

The title compound was prepared by reaction of α-(1,2,4-triazol-1-yl) acetophenone (5.7 g, 0.02 mol), CS_2 (1.9 g, 0.025 mol) and

$BrCH_2CH_2Br$ (0.025 mol) in a diethyl ether solution (40 ml) at room temperature. Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from chloroform–ethyl acetate (*v*/*v*, 1:3) at room temperature.

Crystal data

$C_{13}H_{11}N_3OS_2$	D_x = 1.486 Mg m^{-3}
M_r = 289.37	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 20 reflections
a = 8.0523 (16) Å	θ = 2–11°
b = 10.170 (2) Å	μ = 0.41 mm^{-1}
c = 17.116 (5) Å	T = 293 (2) K
β = 112.63 (3)°	Block, yellow
V = 1293.8 (6) Å^3	0.20 × 0.20 × 0.18 mm
Z = 4	

Data collection

Rigaku R-AXIS IV imaging-plate diffractometer	1868 reflections with $I > 2\sigma(I)$
	R_{int} = 0.036
φ scans	θ_{max} = 26.5°
Absorption correction: none	$h = 0 \rightarrow 10$
4447 measured reflections	$k = -13 \rightarrow 12$
2642 independent reflections	$l = -22 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 0.668P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.047	
$wR(F^2)$ = 0.103	
S = 1.09	$(\Delta/\sigma)_{max} < 0.001$
2642 reflections	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
172 parameters	$\Delta\rho_{min}$ = −0.40 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected torsion angles (°).

C5—C6—C7—C8	47.1 (5)	N2—N3—C8—C9	−98.4 (3)
N2—N3—C8—C7	78.5 (4)	S2—C9—C8—C7	−179.6 (2)
S1—C9—C8—C7	3.2 (5)	C1—C6—C7—O1	41.3 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10B···O1^{i}	0.97	2.58	3.422 (4)	146
C11—H11B···N2^{i}	0.97	2.60	3.559 (4)	170
C13—H13A···N2^{ii}	0.93	2.49	3.359 (4)	156

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

The H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H distances in the range 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

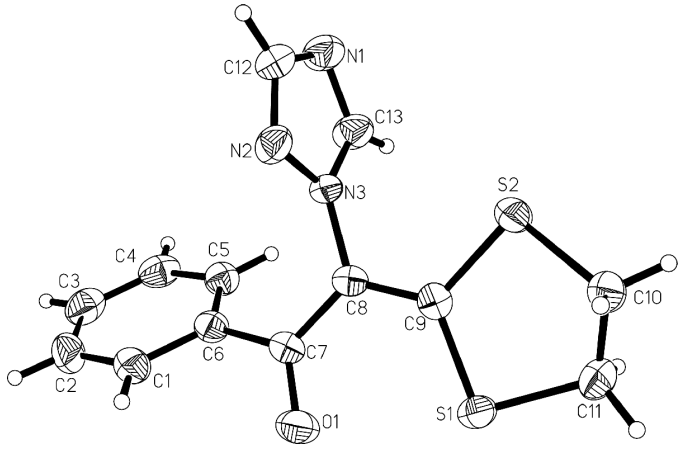


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

Data collection: *R-AXIS Software* (Rigaku, 1997); cell refinement: *R-AXIS Software*; data reduction: *R-AXIS Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL*/*PC* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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