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4,4-Dimethyl-3-oxo-1-(1,2,4-triazol-1-yl)-pentan-2-yl *N,N*-dimethyldithiocarbamate

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Key indicators

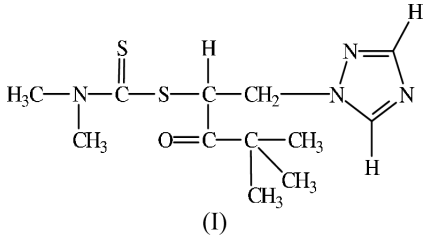
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.045
wR factor = 0.114
Data-to-parameter ratio = 18.1

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

In the title compound, $C_{12}H_{20}N_4OS_2$, the dihedral angle between the plane of the *N,N*-dimethyldithiocarbamate group and the plane of the triazole moiety is 9.96 (2)°. There are weak C—H···N intermolecular interactions in the crystal structure, contributing to its stability.

Comment

As an important type of fungicides, triazole compounds are highly efficient and of low toxicity (Xu, Zhang *et al.*, 2002; Xu, Lu *et al.*, 2002; Zhao *et al.*, 1998). At present, studies on triazole derivatives are mainly concentrated on compounds with triazole as the only active group. Reports of triazole compounds that contain both a triazole and another active group in a single molecule have rarely appeared. Dialkyl-substituted dithiocarbamate salts have also shown interesting biological effects (Gringeri *et al.*, 1988). *N,N*-Dialkyldithiocarbamates have been known as broad-range fungicides and they have a different fungicidal mechanism from triazole compounds (Xu, Jiao *et al.*, 2002). However, triazole compounds containing *N,N*-dimethyldithiocarbamate groups have rarely been reported. In order to search for new triazole compounds with higher bioactivity, the title compound, (I), was synthesized.



(I)

In the title compound, (I), the bond lengths and angles are normal in the *tert*-butyl group and triazole ring (Xue *et al.*, 2000; Liu *et al.*, 2002). The bond lengths and angles in the *N,N*-dimethyldithiocarbamate group are in good agreement with an earlier report (Jian *et al.*, 1999). Atom C10 lies in the triazole ring (N2/N3/N4/C11/C12) plane, and the deviations from the least-squares plane through the ring atoms are all smaller than 0.022 (3) Å. All atoms of the *N,N*-dimethyldithiocarbamate group lie in a plane, and the largest deviation from the least-squares plane is 0.014 (3) Å. The dihedral angle between the plane of the *N,N*-dimethyldithiocarbamate group and the plane of the triazole moiety is 9.96 (2)°.

The packing is stabilized by weak C—H···N hydrogen-bond interactions (Table 2) (Steiner, 1996; Jeffrey *et al.*, 1985).

Experimental

The title compound was prepared by reaction of *tert*-butyl 1-bromo-2-(1,2,4-triazol-1-yl)ethyl ketone with a chloroform solution of 2,2-dimethyl-4-(*N,N*-dimethyldithiocarbamato)sodium. Single crystals of the title compound suitable for X-ray measurements were obtained by recrystallization from ethyl ethanoate/cyclohexane (*v*/*v* = 1:3) at room temperature.

Crystal data

$C_{12}H_{20}N_4OS_2$	D_x = 1.221 Mg m^{-3}
M_r = 300.44	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 20 reflections
a = 12.315 (3) Å	θ = 2–11°
b = 12.057 (2) Å	μ = 0.32 mm^{-1}
c = 12.532 (3) Å	T = 293 (2) K
β = 118.55 (3)°	Pillar, colorless
V = 1634.5 (8) Å^3	0.25 × 0.20 × 0.15 mm
Z = 4	

Data collection

Oxford Instruments point-detector diffractometer	θ_{max} = 26.0°
$\omega/2\theta$ scans	$h = -15 \rightarrow 0$
Absorption correction: none	$k = -15 \rightarrow 15$
5132 measured reflections	$l = -13 \rightarrow 16$
3130 independent reflections	3 standard reflections
2189 reflections with $I > 2\sigma(I)$	every 100 reflections
R_{int} = 0.025	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.114	$\Delta\rho_{max}$ = 0.24 e Å^{-3}
S = 1.02	$\Delta\rho_{min}$ = −0.19 e Å^{-3}
3130 reflections	Extinction correction: *SHELXL*97
173 parameters	Extinction coefficient: 0.0164 (16)
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å).

S1—C3	1.780 (2)	O1—C5	1.205 (3)
S1—C4	1.810 (2)	N2—N3	1.357 (3)
S2—C3	1.651 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···S2	0.96	2.45	2.995 (3)	116
C2—H2A···S1	0.96	2.24	2.831 (3)	119
C4—H4B···S2	0.98	2.57	3.154 (2)	118

H atoms were positioned geometrically and were treated as riding on their parent C atoms, with C—H = 0.93—0.96 Å and U_{iso}(H) = 1.2 or 1.5 times U_{eq}(C).

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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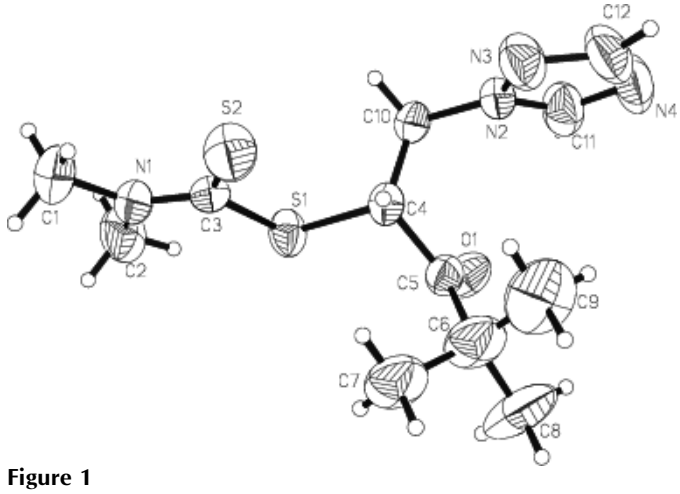

Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

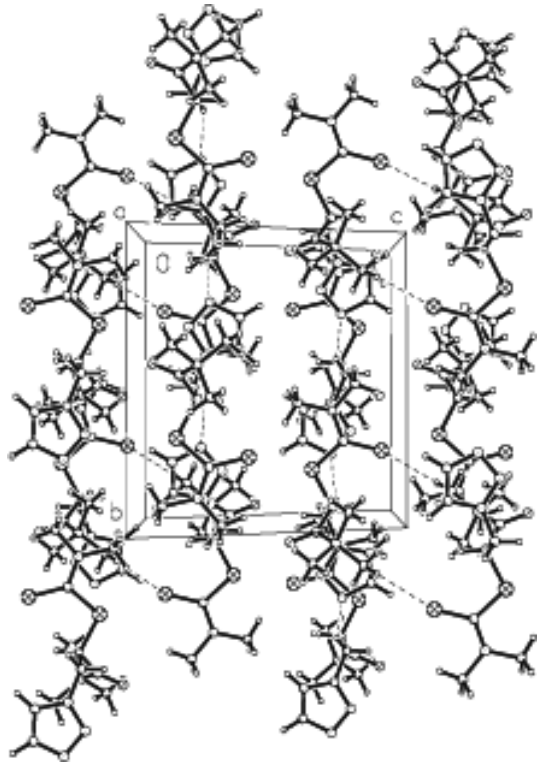

Figure 2
The packing of the title compound. Hydrogen bonds are shown as dashed lines.

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