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2-[(*p*-Methoxyphenylcarbonyl)(1,2,4-triazol-1-yl)methyl]sulfanyl-4,6-dimethylpyrimidine

Fangfang Jian,* Hailian Xiao and Liangzhong Xu

New Materials and Function, Coordination Chemistry Laboratory, Qingdao University of Science and Technology, Qingdao 266042, Peoples Republic of China

Correspondence e-mail: ffj2003@163169.net

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.125
Data-to-parameter ratio = 14.3

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

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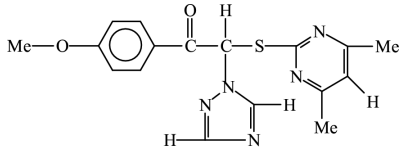
In the title compound, $C_{17}H_{17}N_5O_2S$, the dihedral angles between the plane of the 4,6-dimethyl-2-mercaptopyrimidine group and the plane of the triazole and *p*-methoxyphenylcarbonyl groups are 79.64 (2) and 0.44 (2)°, respectively. There are weak C—H···O and C—H···N intermolecular interactions between the molecules in the crystal lattice.

Comment

As an important type of fungicides, triazole compounds are highly efficient, of low toxicity and capable of being absorbed through the stomach and intestines (Anderson, 1982; Shi *et al.*, 1995; Xu *et al.*, 2002). At present, the studies on triazole derivatives are mainly concentrated on compounds with triazole as the only active group. Reports of triazole compounds containing both a triazole group and another active group in a single molecule are rare. Some pyrimidines have been used as highly efficient fungicides of low toxicity (Tang & Li, 1998) in the control of powdery mildew. In this paper, we report the single-crystal structure of the title compound, (I).



(I)

In (I), the bond lengths and angles are generally normal in the phenyl ring and the triazole ring (Ji *et al.*, 2002; Liu *et al.*, 2002). The bond lengths and angles in the 4,6-dimethyl-2-mercaptopyrimidine group are in good agreement with an earlier report (Low *et al.*, 2002). Atom C9 of the central chain lies in the triazole ring (N1/N2/C11/N3/C10) plane, and the deviation from the least-squares plane through the ring atoms is smaller than 0.023 (3) Å. The atoms of the central chain (C5/C8/O2/C9/S1/C12) are almost planar, with a maximum displacement of 0.236 (2) Å for C12. The dihedral angles formed by the pyrimidine, phenyl and triazole planes with the central chain (C5/C8/O2/C9/S1/C12) are 9.85 (4), 10.29 (6) and 80.70 (8)°, respectively. The methoxy O1 and carbonyl C8 atoms lie in the C2–C7 phenyl plane, and the largest deviation from the least-squares plane through the ring atoms is 0.026 (3) Å. The dihedral angle between the triazole ring moiety and the phenyl ring is 79.22 (2)°. Nine non-H atoms in the 4,6-dimethyl-2-mercaptopyrimidine group are also reasonably coplanar, and the largest deviation from the least-squares plane is 0.021 (3) Å. This plane is nearly parallel to the plane of the *p*-methoxyphenylcarbonyl group, with a dihedral

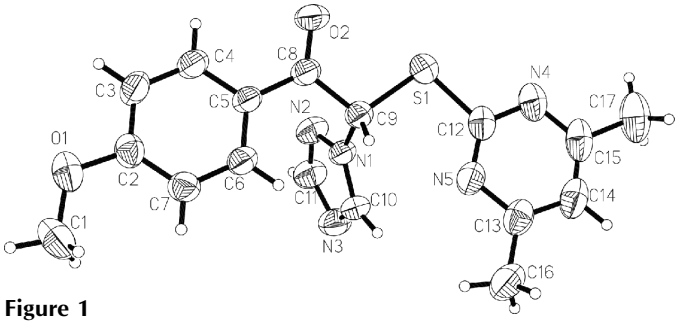


Figure 1
The structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

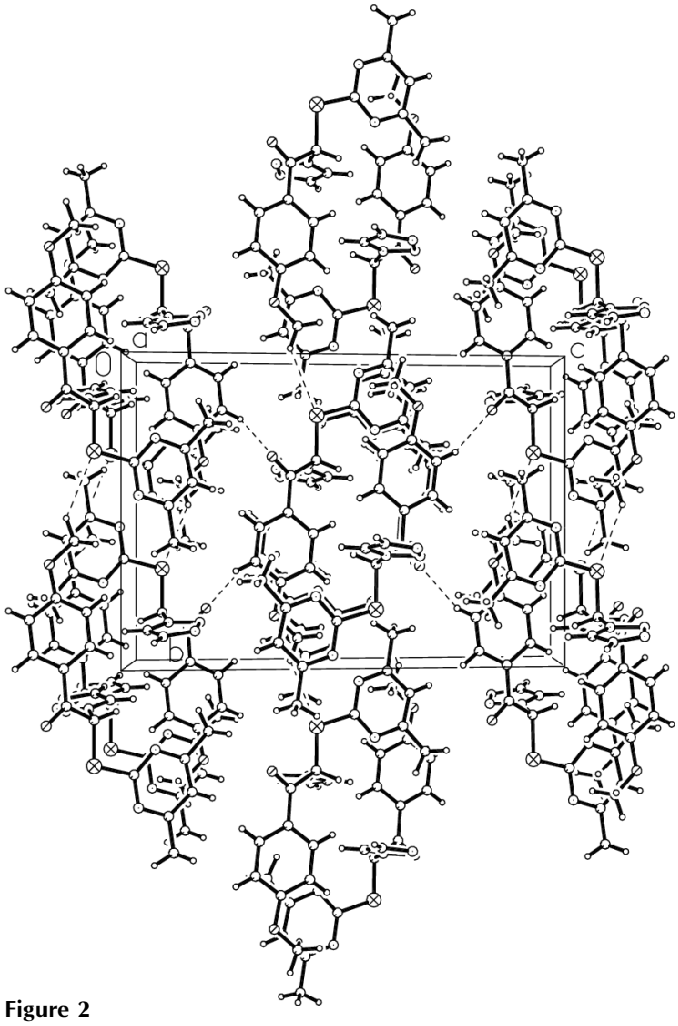


Figure 2
A view of the packing of the title compound.

angle of 0.44 (2)°. The dihedral angle between the plane of the 4,6-dimethyl-2-mercaptopyrimidine group with the plane of the triazole moiety is 79.64 (2)°.

Packing is stabilized by weak C—H···O and C—H···N interactions (Table 2) (Steiner, 1996; Jeffrey *et al.*, 1985).

Experimental

The title compound was prepared by reaction of (1,2,4-triazol-1-yl)(*ρ*-methoxyphenylcarbonyl)methane with 4,6-dimethyl-2-thioetherpyrimidine in chloroform. 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

$C_{17}H_{17}N_5O_2S$
M_r = 355.42
Monoclinic, $P2_1/c$
a = 8.0158 (16) Å
b = 12.462 (3) Å
c = 17.824 (4) Å
β = 99.89 (3)°
V = 1754.0 (7) Å^3
Z = 4
D_x = 1.346 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 20 reflections
θ = 2–11°
μ = 0.21 mm^{-1}
T = 293 (2) K
Pillar, yellow
0.25 × 0.20 × 0.15 mm

Data collection

Oxford Instruments point-detector diffractometer
$\theta/2\theta$ scans
Absorption correction: none
5553 measured reflections
3257 independent reflections
2334 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.9°
$h = -9 \rightarrow 9$
$k = 0 \rightarrow 15$
$l = -21 \rightarrow 21$
3 standard reflections
every 100 reflections
intensity decay: 0.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.04
3257 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0696P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0062 (12)

Table 1
Selected geometric parameters (Å).

S1—C12	1.775 (3)	O1—C1	1.429 (3)
S1—C9	1.816 (2)	O2—C8	1.215 (3)
O1—C2	1.364 (3)	N1—N2	1.368 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3B···O2^{i}	0.93	2.52	3.409 (2)	159
C6—H6A···N3^{ii}	0.93	2.57	3.340 (3)	139
C9—H9A···N5	0.98	2.47	2.840 (3)	102
C10—H10A···N5	0.93	2.58	3.054 (3)	111

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

The H atoms were fixed geometrically and were treated as riding on the parent C atoms, with C—H distances in the range 0.93–0.98 Å. U_{iso}= 1.2 and 1.5 times U_{eq} of the parent atom.

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* (Sheldrick, 1990); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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