# 4-{2-[(4-Methoxyphenyl)sulfanyl]-2-(1,2,3-thiadiazol-4-yl)acetyl}morpholine

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Key indicators

Single-crystal X-ray study
$T = 294$ K
Mean σ(C–C) = 0.005 Å
R factor = 0.050
wR factor = 0.145
Data-to-parameter ratio = 14.0

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

In the title molecule, $C_{15}H_{17}N_3O_3S_2$, the morpholine ring adopts a chair conformation. The benzene and the thiadiazole rings make a dihedral angle of 30.9 (4)°. The crystal packing is stabilized by van der Waals forces.

Comment

It is known that 1,2,3-thiadiazole derivatives have good biological activities (Thomas *et al.*, 1985); for instance, 1,2,3-thiadiazole-5-formamides exhibit excellent fungicidal activity (Tsubata *et al.*, 1999). We became interested in synthesizing 1,2,3-thiadiazoleacetamide analogues of the lead 1,2,3-thiadiazole-4-formamide, due to their high fungicidal activity. Here we present the crystal structure of the title compound, (I), which has been determined during a search for relationships between the structure and fungicidal activity of the above derivatives.

(I)
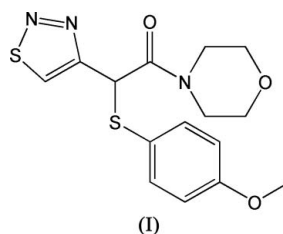
In (I) (Fig. 1), all bond lengths and angles (Table 1) show normal values. The morpholine ring adopts a chair conformation (Table 1). The benzene and the thiadiazole rings make a dihedral angle of 30.9 (4)°. The crystal packing is stabilized by van der Waals forces.

Experimental

Compound (I) was prepared according to the reported precedure of Zhao *et al.* (2003), using α-chloro-1,2,3-thiadiazole-4-acetylmorpholine (4 mmol), 4-methoxybenzenethiol (4 mmol), potassium carbonate (5 mmol) and acetonitrile (15 ml) (1.07 g, 76% yield). Colourless single crystals suitable for X-ray diffraction analysis were obtained by recrystallization from methanol.

Crystal data

$C_{15}H_{17}N_3O_3S_2$	$Z = 2$
$M_r = 351.44$	$D_x = 1.392$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.680$ (4) Å	Cell parameters from 2133
$b = 10.118$ (5) Å	reflections
$c = 11.339$ (5) Å	$\theta = 2.8–26.2°$
$\alpha = 83.092$ (8)°	$\mu = 0.34$ mm^{-1}
$\beta = 68.493$ (6)°	$T = 294$ (2) K
$\gamma = 64.905$ (7)°	Prism, colourless
$V = 838.3$ (7) Å^3	$0.18 \times 0.14 \times 0.10$ mm

organic papers

Bruker SMART CCD area-detector diffractometer

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)

$T_{min} = 0.926$, $T_{max} = 0.967$

4274 measured reflections

2934 independent reflections

2300 reflections with $I > 2\sigma(I)$

$R_{int} = 0.017$

$\theta_{max} = 25.0°$

$h = -9 \rightarrow 10$

$k = -7 \rightarrow 12$

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.050$

$wR(F^2) = 0.145$

$S = 1.05$

2934 reflections

210 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2 + 0.7187P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.77$ e Å^{-3}

$\Delta\rho_{min} = -0.31$ e Å^{-3}

Extinction correction: *SHELXL97*

Extinction coefficient: 0.083 (7)

Figure 1
The molecular structure of (I), showing displacement ellipsoids at the 30% probability level.

Table 1
Selected geometric parameters (Å, °).

S1—N1	1.677 (3)	N1—N2	1.306 (4)
S1—C1	1.681 (3)	N2—C2	1.370 (4)
S2—C9	1.777 (3)		
C9—S2—C3	101.16 (12)	N3—C4—C3	117.6 (2)
C2—C3—C4	114.3 (2)		
N2—C2—C3—C4	−144.2 (3)	C9—S2—C3—C2	−74.8 (2)
N2—C2—C3—S2	95.7 (3)	C2—C3—C4—N3	159.1 (3)

H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93 (aromatic), 0.97 (methylene), 0.98 (methine) or 0.96 Å (methyl), and with $U_{iso}(H) = 1.2$–$1.5\ U_{eq}(C)$.

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, 1998); software used to prepare material for publication: *SHELXTL*.
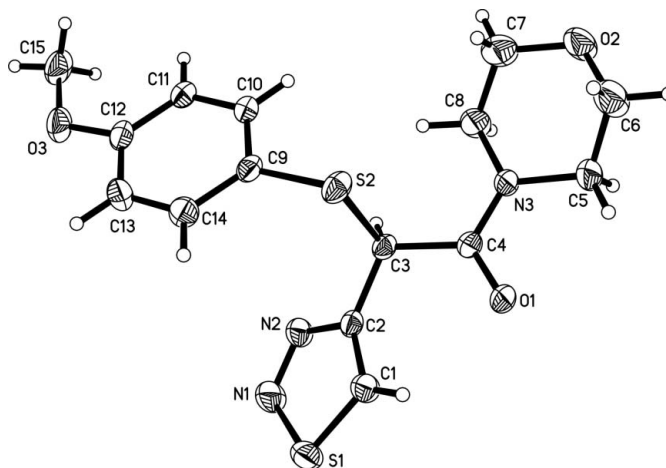
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