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2-(4-Fluorophenyl)-3-[5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl]thiazolidin-4-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.053
wR factor = 0.146
Data-to-parameter ratio = 14.6

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

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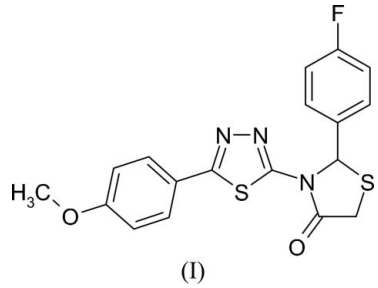
In the title compound, $C_{18}H_{14}FN_3O_2S_2$, the thiazolidine ring adopts an envelope conformation. There are intramolecular C—H···S and intermolecular C—H···O interactions, forming chains along the *b* axis.

Comment

Thiadiazole derivatives containing the thiazolidinone unit are of great interest because of their chemical and pharmaceutical properties. Some derivatives have fungicidal activities and exhibit some herbicidal activities (Chen *et al.*, 2000; Kidwai *et al.*, 2000; Vicentini *et al.*, 1998), and some show insecticidal activities (Arun *et al.*, 1999; Wasfy *et al.*, 1996).



(I)

We are focusing our synthetic and structural studies on thiadiazole derivatives and we have published recently the structure of 3-[5-(4-fluorophenyl)-1,3,4-thiadiazol-2-yl]-2-phenylthiazolidin-4-one (Wan *et al.*, 2006). We report the crystal structure of a close analog, (I), in which the 4-fluorophenyl substituent is replaced by 4-methoxyphenyl, and 2-phenyl is replaced by 4-fluorophenyl. In (I), the thiazolidine ring adopts an envelope conformation with atom C7 at the tip of the flap (Fig. 1 and Table 1). There are intramolecular C—H···S and intermolecular C—H···O interactions (Table 2), forming chains along the *b* axis (Fig. 2).

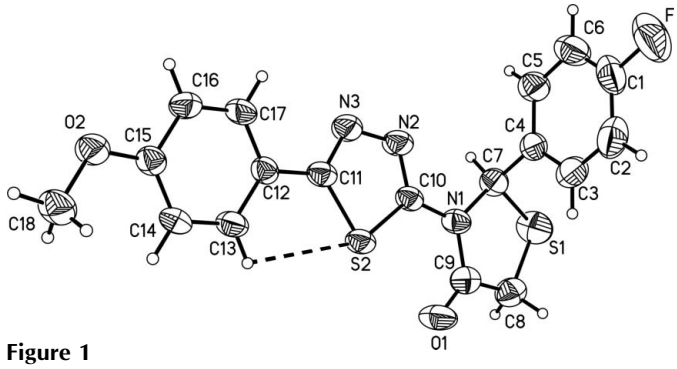


Figure 1
A view of the molecular structure of (I), showing atom displacement ellipsoids at the 50% level. The dashed line indicates a C—H···S interaction.

Experimental

(4-Fluorobenzylidene)[5-(4-methoxyphenyl)-1,3,4-thiadiazol-2-yl]-amine (5 mmol) and 3-mercaptopropionic acid (5 mmol) were dissolved in toluene (50 ml). The resulting water was removed by distillation over a period of 5 h. The reaction mixture was left to cool to room temperature and filtered; the solid was recrystallized from acetone to give (I) (yield 81.3%, m.p. 520–524 K). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of an acetone solution.

Crystal data

$C_{18}H_{14}FN_3O_2S_2$
M_r = 387.44
Monoclinic, $C2/c$
a = 17.750 (4) Å
b = 6.3720 (13) Å
c = 31.761 (6) Å
β = 101.55 (3)°
V = 3519.5 (12) Å^3
Z = 8
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 298 K
Block, colorless
0.40 × 0.40 × 0.30 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.879, T_{max} = 0.907
3562 measured reflections
3449 independent reflections
2562 reflections with $I > 2\sigma(I)$
R_{int} = 0.089
θ_{max} = 26.0°
3 standard reflections
every 200 reflections
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.146
S = 1.11
3449 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0642P)^2 + 4.2621P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0034 (4)

Table 1
Selected torsion angles (°).

C9—N1—C7—S1	9.3 (3)	C7—N1—C9—C8	−5.7 (4)
C8—S1—C7—N1	−8.0 (2)	S1—C8—C9—N1	−1.2 (3)
C7—S1—C8—C9	5.5 (2)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O1^{i}	0.98	2.49	3.299 (4)	140
C13—H13A···S2	0.93	2.77	3.163 (3)	107

Symmetry code: (i) $x, y+1, z$.

All H atoms were placed geometrically, with C—H = 0.93–0.98 Å, and included in the refinement in the riding-model approximation with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

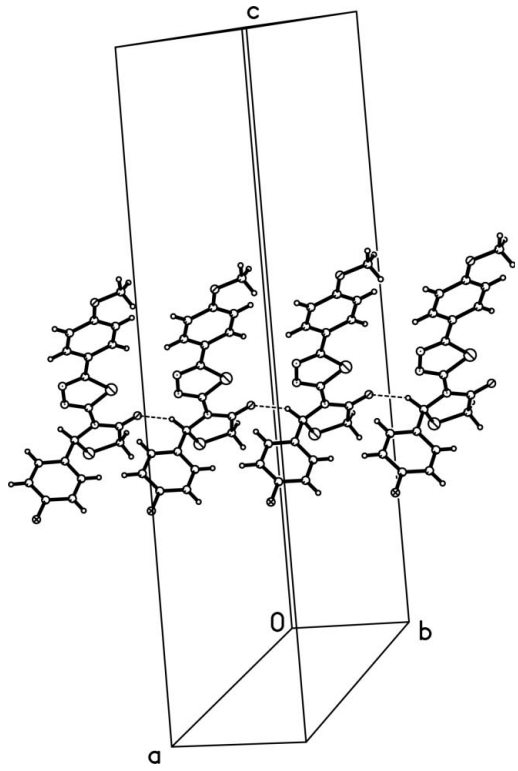


Figure 2
Part of the crystal structure of (I). Dashed lines indicate C—H···O interactions.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

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