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Ethyl 7-methyl-2-[4-(methylsulfanyl)benzylidene]-5-[4-(methylsulfanyl)phenyl]-3-oxo-2,3-dihydro-5*H*-thiazolo[3,2-*a*]pyrimidine-6-carboxylate

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Key indicators

Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.004 Å
R factor = 0.055
wR factor = 0.142
Data-to-parameter ratio = 18.4

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

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The title compound, $C_{25}H_{24}N_2O_3S_3$, was crystallized from a methanol–acetone mixture. The monoclinic structure features one molecule in the asymmetric unit. The crystal packing is stabilized by π stacking.

Comment

Syntheses of a number of thiazolo[3,2-*a*]pyrimidine derivatives are reported in the literature, and these compounds are known to possess anti-inflammatory, anticancer and antimicrobial properties (Tozkoparan *et al.*, 1998; Holla *et al.*, 2004; Sayed *et al.*, 2006).

The structure of the newly synthesized compound, (4), was confirmed by its elemental analysis, and by IR, ^{1}H NMR and mass spectroscopic studies.

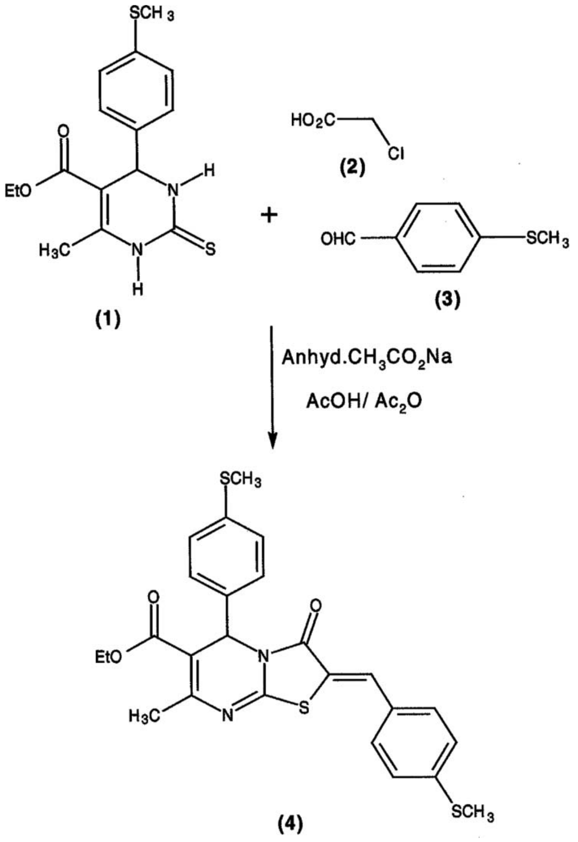

Fig. 1 shows the molecular structure of (4). The geometry is unexceptional; the pyrimidine group and benzene ring C19–C24 are essentially coplanar [dihedral angle 4.73 (8)°]. The dihedral angle between the benzene ring C3–C7 and the pyrimidine group is 73.77 (6)°.

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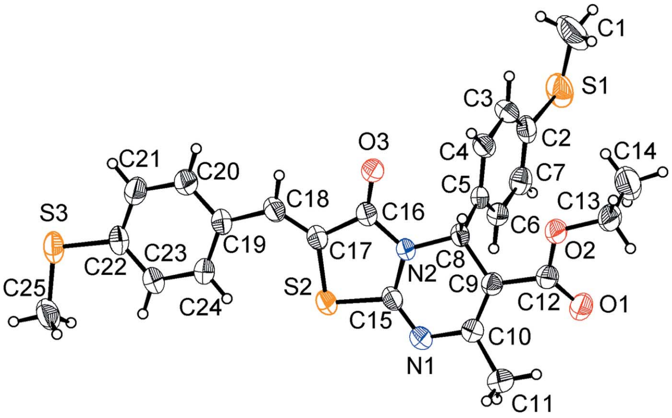

Figure 1
The molecular structure of (4). Displacement ellipsoids are drawn at the 50% probability level.

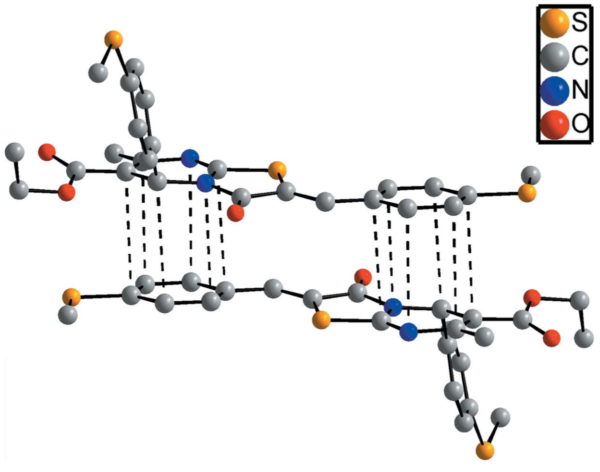

Figure 2
The dimer formed by two inversion-related molecules of (4). π bonds are indicated by dashed lines. The upper molecule is symmetry-related to the lower molecule by ($1 - x$, $2 - y$, $-z$). H atoms have been omitted.

The structure is stabilized by considerable π stacking [Fig. 2; C—C = 3.604 (4)–3.648 (4) Å, C—N = 3.505 (3)–3.657 (4) Å].

Experimental

A mixture of (1) (3.22 g, 0.01 mol), (2) (0.95 g, 0.01 mol), anhydrous sodium acetate (2 g), glacial acetic acid (20 ml), acetic anhydride (15 ml) and (3) (1.52 g, 0.01 mol) were refluxed for 5 h. The progress of the reaction was monitored by thin-layer chromatography. After the completion of the reaction, the resulting mixture was cooled and poured into crushed ice. The solid that separated was filtered off, washed with water, dried and recrystallized from a methanol/acetone (1:1) mixture to give orange crystals (yield 76%, m.p. 423–425 K). Analysis for $C_{25}H_{24}N_2O_3S_3$: found (calculated): C 60.41 (60.46), H 4.89 (4.87), N 5.64 (5.62)%.

IR (KBr, ν, cm^{-1}): 2976 (C—H), 1710 (C═O), 1606 (C═N), 1541 (C═C), 1159(C—O); ^{1}H NMR ($CDCl_3$): δ 1.22 (*t*, 3H, J = 7.12 Hz, ester-CH_3), 4.14 (*q*, 2H, J = 7.12 Hz, ester-CH_2), 2.44 (*s*, 3H, CH_3), 2.51 (*s*, 3H, SCH_3), 6.18 (*s*, 1H, CH), 7.17 (*d*, 2H, J = 8.36 Hz, 4-methylthiophenyl), 7.33 (*d*, 2H, J = 8.32 Hz, 4-methylthiophenyl), 7.23 (*d*, 2H, J = 8.28 Hz, 4-methylthiophenyl), 7.38 (*d*, 2H, J = 8.36 Hz, 4-methylthiophenyl), 7.71 (*s*, 1H, exocyclic CH).

Crystal data

$C_{25}H_{24}N_2O_3S_3$
M_r = 496.67
Monoclinic, $P2_1/n$
a = 8.771 (1) Å
b = 12.384 (2) Å
c = 22.224 (6) Å
β = 95.47 (2)°
V = 2403.1 (8) Å^3
Z = 4
D_x = 1.373 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 297 K
Block, orange
0.32 × 0.19 × 0.14 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: none
27621 measured reflections
5484 independent reflections
3683 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.098
$\theta_{\rm max}$ = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.142
S = 1.05
5484 reflections
298 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 1.7062P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.001
$\Delta\rho_{\rm max}$ = 0.34 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.35 e Å^{-3}

All H atoms were placed in calculated positions with a C—H bond distance of 0.96 for methyl, 0.93 for aromatic and 0.98 for tertiary H atoms. They were refined with an isotropic displacement parameter of 1.5 (methyl) or 1.2 (all others) times $U_{\rm eq}$ of their respective carrier atom. The methyl groups were allowed to rotate to best fit the experimental electron density. No explicit absorption correction was applied, but using *EVALCCD* (Duisenberg *et al.*, 2003) the data were corrected using an error model based on the procedure of McCandlish *et al.* (1975), thus partially accounting for absorption effects.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DIRAX/LSQ* (Duisenberg, 1992); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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References

Brandenburg, K. (2006). *DIAMOND*. Release 3.1d. Crystal Impact GbR, Bonn, Germany.
Duisenberg, A. J. M. (1992). *J. Appl. Cryst.* **25**, 92–96.
Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.
Holla, B. S., Rao, B. S., Sarojini, B. K. & Akberali, P. M. (2004). *Eur. J. Med. Chem.* **39**, 777–783.
McCandlish, L. E., Stout, G. H. & Andrews, L. C. (1975). *Acta Cryst.* A**31**, 245–249.
Nonius (1999). *COLLECT*. Nonius BV, Delft, The Netherlands.
Sayed, H. H., Shamroukh, A. H. & Rashad, A. E. (2006). *Acta Pharm.* **56**, 231–244.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tozkoparan, B., Ertan, M., Krebs, B., Lage, M., Kelicen, P. & Demirdamar, R. (1998). *Arch. Pharm. Pharm. Med. Chem.* **331**, 201–206.
Westrip (2007). *publCIF*. In preparation.