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3-(4-Ethoxyphenyl)-6-(4-methoxyphenyl)-7*H*-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazine

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.136
Data-to-parameter ratio = 13.4

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

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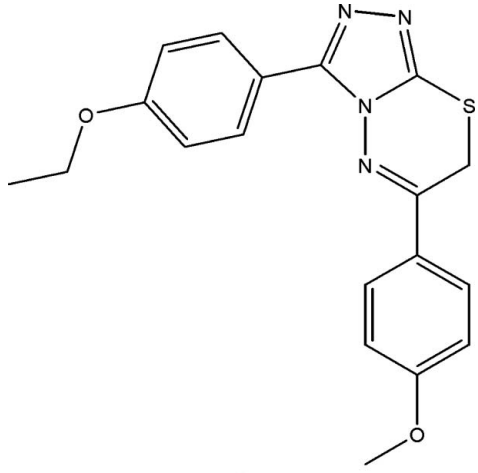
The title compound, $C_{19}H_{18}N_4O_2S$, was prepared by the reaction of 4-amino-3-(4-ethoxyphenyl)-5-mercapto-1,2,4-triazole and 2-bromo-4′-methoxyacetophenone. The bond lengths and angles show normal values. The triazole ring makes dihedral angles of 5.7 (1) and 8.6 (1)° with the two benzene rings.

Comment

1,2,4-Triazoles fused with six-membered ring systems are found to have diverse applications in the fields of medicine, agriculture and industry. The commonly known systems are triazoles fused with pyridine, pyridazine, pyrimidine, pyrazines and triazines. A literature survey reveals that there are few examples of triazoles fused with thiadiazines. A large number of triazolothiazines have been shown to exhibit antimicrobial (Feng *et al.*, 1992) and diuretic (Mohan & Anjaneyulu, 1987) properties, and act as photographic couplers (Holla *et al.*, 2001). We report here the synthesis and crystal structure of the title compound, (I), which contains the diazine ring system with attached 4-ethoxyphenyl and 4-methoxyphenyl groups (Fig. 1).



(I)

In (I), the bond lengths and angles (Table 1) are usual. The triazole and two benzene rings are essentially planar, while the six-membered thiadiazine ring (N1/N2/C8/C9/C10/S1) is distorted from planarity and may be regarded as having a screw–boat conformation, with an r.m.s. deviation of 0.251 Å. Atoms C9 and S1 deviate from the thiadiazine mean plane by −0.401 (2) and 0.330 (1) Å, respectively. In the thiadiazine ring, the S—C and C—N bond lengths are comparable to those observed in related compounds (Sert *et al.*, 2003; Zou *et*

al., 2004). The C and N atoms involved in the conjugated form of the triazole ring show normal bond lengths (Allen *et al.*, 1987; Jin *et al.*, 2004; Table 1). The triazole ring makes dihedral angles of 5.7 (1) and 8.6 (1)°, respectively, with the C2–C7 and C12–C17 benzene rings.

Experimental

4-Amino-3-(4-ethoxyphenyl)-5-mercapto-1,2,4-triazole was prepared from 4-ethoxybenzoic acid hydrazide, whose starting material was 4-ethoxybenzoic acid, following the literature method of Zhang *et al.* (1990). To a solution of 4-amino-3-(4-ethoxyphenyl)-5-mercapto-1,2,4-Trizole (0.001 mol) in absolute ethanol was added 2-bromo-4-methoxyacetophenone (0.001 mol). The mixture was refluxed for 7 h. The solid obtained on cooling was filtered off, washed with cold water, dried and recrystallized from ethanol to give compound (I). The purified product was dissolved in 95% ethanol and kept at room temperature for 5 d and colourless single crystals of (I) were formed (m.p. 474–475 K).

Crystal data

$C_{19}H_{18}N_4O_2S$
M_r = 366.43
Monoclinic, $P2_1/c$
a = 11.1834 (8) Å
b = 13.7038 (10) Å
c = 15.8307 (9) Å
β = 133.270 (3)°
V = 1766.5 (2) Å^3
Z = 4
D_x = 1.378 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3578 reflections
θ = 2.5–25.0°
μ = 0.21 mm^{-1}
T = 298 (2) K
Block, colourless
0.39 × 0.36 × 0.28 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.914, T_{max} = 0.935
9261 measured reflections
3175 independent reflections
2829 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 25.2°
$h = -12 \rightarrow 13$
$k = -16 \rightarrow 10$
$l = -17 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.136
S = 1.12
3175 reflections
237 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2 + 0.4697P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C10	1.734 (2)	N2—C11	1.383 (2)
S1—C9	1.807 (2)	N3—C10	1.301 (3)
N1—C8	1.289 (3)	N3—N4	1.391 (3)
N1—N2	1.390 (2)	N4—C11	1.307 (3)
N2—C10	1.370 (3)		
C10—S1—C9	95.03 (10)	C10—N2—N1	128.46 (17)
C8—N1—N2	116.54 (17)	C10—N3—N4	106.87 (18)
C10—N2—C11	105.17 (17)	C11—N4—N3	108.63 (18)

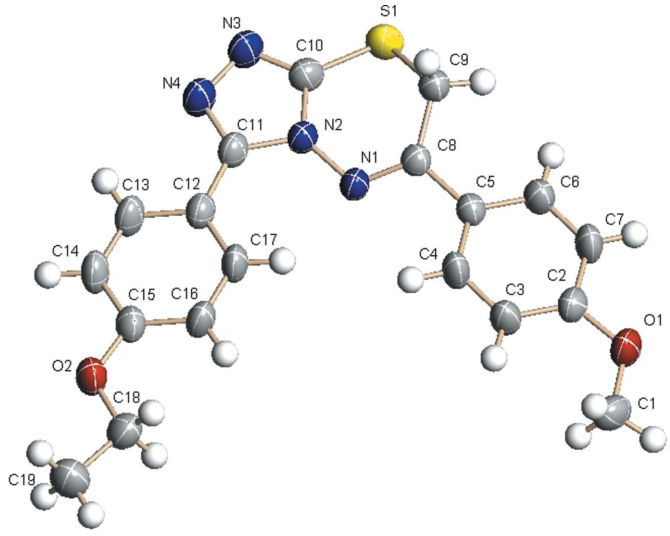


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and displacement ellipsoids at the 30% probability level.

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with Csp^2—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C), and Csp^3—H = 0.96 or 0.97 Å and U_{iso}(H) = 1.5U_{eq}(C).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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, 2002); software used to prepare material for publication: *SHELXL97*.

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