Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(2-Ethoxyphenyl)-6-phenyl-1,2,4-triazolo-[3,4-*b*][1,3,4]thiadiazole

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.116
Data-to-parameter ratio = 13.3

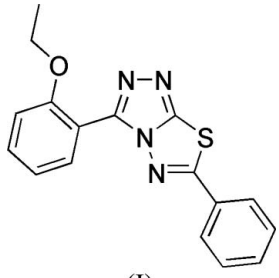
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 June 2005
Accepted 15 June 2005
Online 24 June 2005

In the title compound, $C_{17}H_{14}N_4OS$, the central heterocyclic system formed by the five-membered triazole and thiadiazole rings is planar. The bond lengths within the system indicate some degree of delocalization.

Comment

1,2,4-Triazolo[3,4-*b*][1,3,4]thiadiazoles are condensed heterocyclic compounds combining the properties of triazoles (Feng *et al.*, 2000) and thiadiazoles (Zhao *et al.*, 2001). As a result, these compound show a wide range of biological activities, such as antimicrobial, antiinflammatory, fungicidal, antiviral, herbicidal and plant-growth regulating activity (Zhang *et al.*, 1994).



(I)

The molecule of the title compound, (I), contains a triazole (ring *A*), a thiadiazole (ring *B*), an ethoxybenzene (ring *C*) and a phenyl ring (ring *D*). All rings are essentially planar, with average deviations from planarity of 0.0017 (2), 0.0055 (2), 0.0054 (3) and 0.0046 (3) Å for rings *A*, *B*, *C* and *D*, respectively. The central heterocyclic system is planar, as indicated by the dihedral angle between rings *A* and *B* [1.05 (6)°] and by the sum of the bond angles around the atoms at the junction of the five-membered rings (360.0 for both N2 and C8). Ring *D* is almost coplanar with the thiadiazole ring [dihedral angle = 3.31 (7)°], while ring *C* is rotated by 49.67 (7)° with respect to the triazole ring.

Bond lengths and angles within the heterocyclic system (Table 1) agree well with the values reported in the literature (Fornies-Marquina *et al.*, 1974; Molina *et al.*, 1989; Zhang *et al.*, 1996; Chen *et al.*, 2000; Dong *et al.*, 2002). The bond lengths indicate some degree of delocalization around the ring system, with the three C=N bonds averaging 1.302 (3) Å and the N—N bonds ranging from 1.375 (2) to 1.404 (3) Å.

Experimental

The title compound was prepared in 80% yield from 4-amino-(2-ethoxyphenyl)-5-mercapto-1,2,4-triazole (5.0 mmol) and benzoic acid

(5.5 mmol) in phosphorus oxychloride (20 ml). The mixture was refluxed for 7 h. The reaction mixture was poured into crushed ice gradually with stirring. Solid potassium hydroxide was added till the pH value was 8. After standing overnight the separated solid was filtered off, washed with cold water, dried, and recrystallized from absolute ethanol to afford the title compound. Single crystals suitable for X-ray data collection were obtained by slow evaporation of an ethanol solution (m.p. 443–445 K). IR (KBr): 3076, 1604, 1528, 1468, 1252, 681 cm^{-1}. ^1H NMR (chloroform-*d*, p.p.m.): 7.89–7.06 (*m*, 9H), 4.17 (*q*, 2H, *J* = 7.0 Hz), 1.30 (*t*, 3H, *J* = 7.0 Hz).

Crystal data

$C_{17}H_{14}N_4OS$	D_x = 1.380 Mg m^{-3}
M_r = 322.38	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 2865 reflections
a = 10.3988 (9) Å	θ = 2.4–24.5°
b = 8.7056 (8) Å	μ = 0.22 mm^{-1}
c = 17.5354 (16) Å	T = 298 (2) K
β = 102.184 (2)°	Block, colorless
V = 1551.7 (2) $Å^3$	0.38 × 0.26 × 0.17 mm
Z = 4	

Data collection

Bruker APEX area-detector diffractometer	2792 independent reflections
	2405 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.026
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	θ_{max} = 25.2°
	$h = -12 \rightarrow 7$
T_{min} = 0.922, T_{max} = 0.964	$k = -10 \rightarrow 10$
8034 measured reflections	$l = -19 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2 + 0.6118P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	
$wR(F^2)$ = 0.116	
S = 1.04	$(\Delta/\sigma)_{max}$ = 0.001
2792 reflections	$\Delta\rho_{max}$ = 0.24 e $Å^{-3}$
210 parameters	$\Delta\rho_{min}$ = −0.23 e $Å^{-3}$
H-atom parameters constrained	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.063 (3)

Table 1
Selected geometric parameters (Å, °).

S1—C8	1.725 (2)	N2—C8	1.359 (2)
S1—C7	1.770 (2)	N2—C9	1.371 (2)
O1—C11	1.362 (2)	N3—C8	1.302 (3)
O1—C16	1.432 (3)	N3—N4	1.404 (3)
N1—C7	1.295 (2)	N4—C9	1.310 (3)
N1—N2	1.375 (2)		
C7—N1—N2	108.20 (16)	N1—C7—S1	116.13 (15)
C8—N2—C9	105.68 (16)	N3—C8—N2	111.76 (19)
C8—N2—N1	118.56 (16)	N3—C8—S1	139.18 (17)
C9—N2—N1	135.76 (16)	N2—C8—S1	109.05 (15)
C8—N3—N4	105.05 (17)	N4—C9—N2	108.21 (18)
C9—N4—N3	109.30 (17)	N4—C9—C10	126.27 (18)
N1—C7—C4	123.43 (18)	N2—C9—C10	125.52 (17)

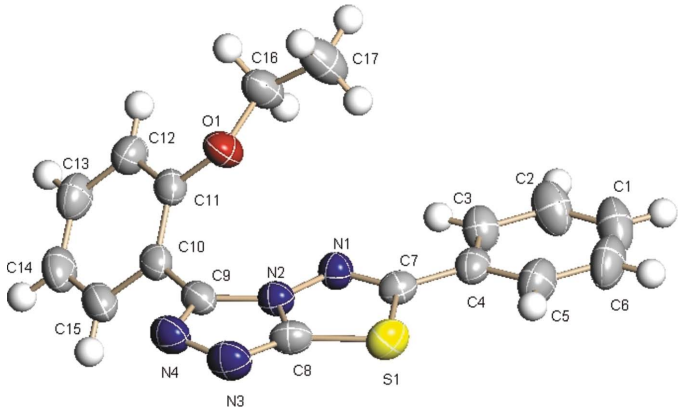


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atom-numbering scheme.

The H atoms were positioned geometrically and allowed to ride on their parent atoms, with C–H = 0.93 Å and U_{iso} = 1.2U_{eq}(C) for aromatic H atoms, and C–H = 0.96–0.97 Å and U_{iso} = 1.5U_{eq}(C) for methylene and methyl H atoms.

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: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge financial support by the Zhejiang Provincial Natural Science Foudation of China (No. M 203149).

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