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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.063
 wR factor = 0.160
Data-to-parameter ratio = 13.2

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

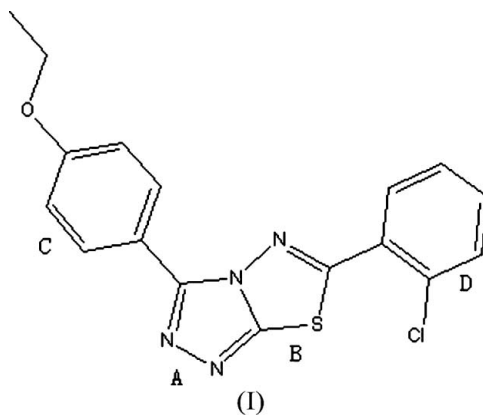
6-(2-Chlorophenyl)-3-(4-ethoxyphenyl)- 1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole

In the title compound, $\text{C}_{17}\text{H}_{13}\text{ClN}_4\text{OS}$, 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. The ethoxybenzene and chlorophenyl rings are located on the same side of the heterocyclic system, resembling the two front claws of a crab.

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Comment

1,2,4-Triazolo[3,4-*b*][1,3,4]thiadiazoles, combining the properties of triazoles (Feng *et al.*, 2000) and thiadiazoles (Zhao *et al.*, 2001), are associated with diverse pharmacological activities, such as antimicrobial, bactericidal, anti-inflammatory, antiviral, antihypertensive, anthelmintic and analgesic activities (Zhang & Chen, 1991; Zhang *et al.*, 1993, 1994; Gupta *et al.*, 1996).



The title compound, (I), contains a triazole ring (A), a thiadiazole ring (B), an ethoxybenzene group (C) and a chlorophenyl group (D). All rings are essentially planar, with average deviations from planarity of 0.0011 (2), 0.0044 (2), 0.0043 (3) and 0.0015 (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 [3.10 (3)°] 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 = 6.70 (3)°], while ring C is rotated by 16.90 (2)° with respect to the triazole ring. The ethoxybenzene and chlorophenyl rings are located on the same side of the heterocyclic system, resembling the two front claws of a crab.

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 1.301 (3) Å and the N—N bonds ranging from 1.369 (3) to 1.404 (4) Å.

Experimental

The title compound was prepared in 78% yield from 4-amino-3-(4-ethoxyphenyl)-5-mercapto-1,2,4-triazole (5.0 mmol) and 2-chlorobenzoic 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.

Crystal data

| | |
|---------------------------------|---|
| $C_{17}H_{15}ClN_4OS$ | $Z = 4$ |
| $M_r = 356.83$ | $D_x = 1.475 \text{ Mg m}^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 10.8298$ (9) Å | $\mu = 0.38 \text{ mm}^{-1}$ |
| $b = 10.6315$ (9) Å | $T = 298$ (2) K |
| $c = 16.6174$ (10) Å | Block, colorless |
| $\beta = 122.870$ (4)° | $0.39 \times 0.21 \times 0.17 \text{ mm}$ |
| $V = 1607.0$ (2) Å ³ | |

Data collection

| | |
|--|--|
| Bruker APEX area-detector diffractometer | 8346 measured reflections |
| φ and ω scans | 2885 independent reflections |
| Absorption correction: multi-scan (SADABS; Bruker, 2002) | 2633 reflections with $I > 2\sigma(I)$ |
| $T_{\min} = 0.866$, $T_{\max} = 0.938$ | $R_{\text{int}} = 0.023$ |
| | $\theta_{\text{max}} = 25.2^\circ$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.0774P)^2 + 0.6007P]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.160$ | $(\Delta/\sigma)_{\text{max}} = 0.002$ |
| $S = 1.20$ | $\Delta\rho_{\text{max}} = 0.33 \text{ e \AA}^{-3}$ |
| 2885 reflections | $\Delta\rho_{\text{min}} = -0.31 \text{ e \AA}^{-3}$ |
| 218 parameters | |
| H-atom parameters constrained | |

Table 1

Selected geometric parameters (Å, °).

| | | | |
|------------|------------|----------|-----------|
| C11—C1 | 1.737 (3) | N1—N2 | 1.369 (3) |
| S1—C8 | 1.729 (3) | N2—C8 | 1.357 (4) |
| S1—C7 | 1.768 (3) | N2—C9 | 1.371 (4) |
| O1—C13 | 1.366 (4) | N3—C8 | 1.301 (4) |
| O1—C16 | 1.428 (4) | N3—N4 | 1.404 (4) |
| N1—C7 | 1.301 (3) | N4—C9 | 1.308 (4) |
| C8—S1—C7 | 88.04 (14) | C8—N2—C9 | 105.7 (2) |
| C13—O1—C16 | 118.1 (2) | N1—N2—C9 | 135.8 (2) |
| C7—N1—N2 | 108.6 (2) | C8—N3—N4 | 104.5 (2) |
| C8—N2—N1 | 118.4 (2) | C9—N4—N3 | 109.9 (2) |

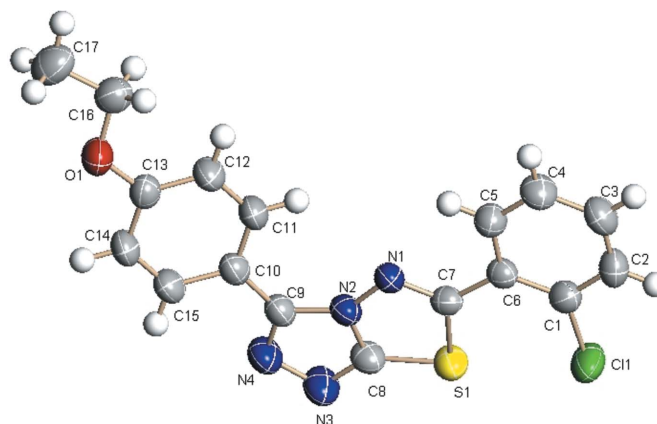


Figure 1

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

All H atoms were positioned geometrically and allowed to ride on their parent atoms with C—H = 0.93 Å, 0.96 or 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ [$1.5U_{\text{eq}}(\text{C})$ for methyl].

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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