Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Xin-Xiang Lei, Xiao-Bo Huang, An-Jiang Zhang* and Li-Xue Zhang

School of Chemistry and Materials Engineering, Wenzhou University, Wenzhou 325027, People's Republic of China

Correspondence e-mail: nmr@wzu.edu.cn

Received 31 August 2006
Accepted 5 September 2006

Key indicators

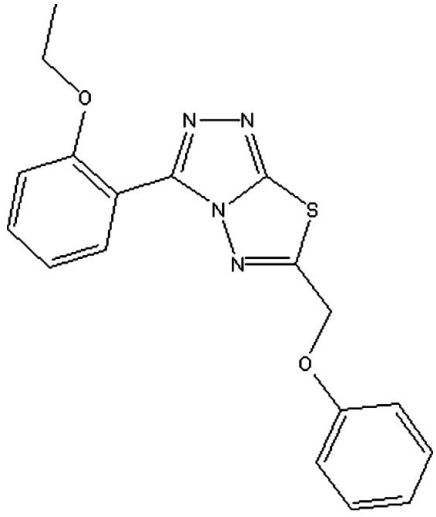
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.053
wR factor = 0.119
Data-to-parameter ratio = 13.6

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

In the title compound, $C_{18}H_{16}N_4O_2S$, 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 possessing 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 *et al.*, 1994; Gupta *et al.*, 1996).



(I)

The molecule of the title compound, (I), contains two five-membered rings, which are essentially coplanar, the dihedral angle between them being 0.6 (3)°. The C1-benzene and C11-benzene rings are twisted with respect to the thiadizaole ring, with dihedral angles of 48.7 (2) and 150.2 (3)°, respectively.

Bond lengths within the heterocyclic system (Table 1) indicate some degree of delocalization and agree with those found in similar structures (Fornies-Marquina *et al.*, 1974; Molina *et al.*, 1989; Zhang *et al.*, 1996; Chen *et al.*, 2000; Dong *et al.*, 2002).

Experimental

Compound (I) was prepared in 81% yield from 4-amino-3-(2-ethoxyphenyl)-5-mercapto-1,2,4-triazole (5.0 mmol) and phenoxyacetic acid (5.5 mmol) in phosphorus oxychloride (20 ml). The reaction mixture was refluxed for 7 h, then poured into crushed ice

gradually with stirring. Solid potassium hydroxide was added until the pH = 8. After being allowed to stand overnight, the precipitate was filtered off, washed with cold water, dried and recrystallized from absolute ethanol to afford single crystals of (I).

Crystal data

$C_{18}H_{16}N_4O_2S$
M_r = 352.41
Monoclinic, $P2_1/n$
a = 10.2328 (9) Å
b = 8.4172 (7) Å
c = 20.2015 (18) Å
β = 98.983 (2)°
V = 1718.6 (3) Å^3
Z = 4
D_x = 1.362 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.21 mm^{-1}
T = 298 (2) K
Rod, colorless
0.22 × 0.21 × 0.20 mm

Data collection

Bruker APEX area-detector diffractometer
φ and ω scans
Absorption correction: none
8831 measured reflections
3086 independent reflections
2560 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 25.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.119
S = 1.09
3086 reflections
227 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.4939P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were positioned geometrically, with C—H = 0.93 (aromatic) or 0.97 Å (methylene), and refined in riding mode, with U_{iso}(H) = 1.2U_{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*.

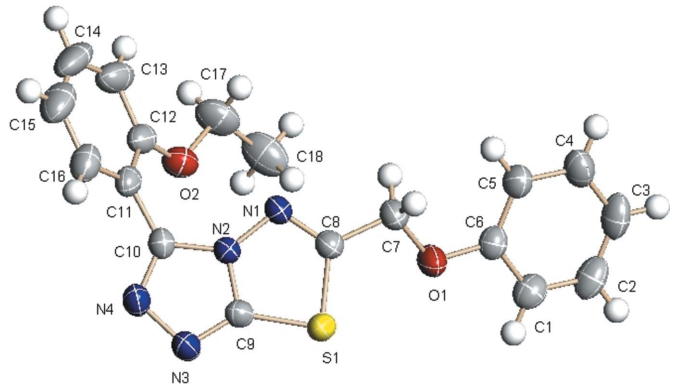


Figure 1
The molecular structure of (I), shown with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

This work was supported by the Zhejiang Provincial Natural Science Foundation of China (No. M203149).

References

Bruker (2002). *SAINT* (Version 6.02), *SMART* (Version 5.62) and *SHELXTL* (Version 6.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Chen, H.-S., Li, Z.-M., Yang, X.-P., Wang, H.-G. & Yao, X.-K. (2000). *Chin. J. Struct. Chem.* **19**, 317–321.
Dong, H.-S., Quan, B., Zhu, D.-W. & Li, W.-D. (2002). *J. Mol. Struct.* **613**, 1–5.
Feng, Zh.-X., Zhang, W.-N., Zhou, Y.-J., Lu, J.-G., Zhu, J. & Li, K. (2000). *Chem. J. Chin. Univ.* **21**, 1221–1226.
Fornies-Marquina, J., Courseille, C. & Elguero, J. (1974). *Cryst. Commun.* **3**, 7–9.
Gupta, R., Sudan, S., Mengi, V. & Kachroo, P. L. (1996). *Indian J. Chem. Sect. B*, **35**, 621–623.
Molina, P., Arques, A., Alias, M. A., Llamos Saiz, A. L. & Foces-Foces, M. C. (1989). *Liebigs Ann. Chem.* pp. 1055–1059.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Zhang, Z.-Y., Zhao, L. & Li, M. (1994). *Chin. J. Org. Chem.* **14**, 74–80.
Zhang, Z.-Y., Zou, N., Zhu, Y., Zhao, L. & Li, M. (1996). *Acta Cryst.* C**52**, 2787–2789.
Zhao, W.-G., Chen, H.-S., Li, Zh.-M., Han, Y.-F., Lai, J.-Y. & Wang, S.-H. (2001). *Chem. J. Chin. Univ.* **22**, 939–942.