Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3,3′-(Butane-1,4-diyldithio)bis(5-phenyl-1,2,4-triazine)

Li-Rong Wen,* Jian-Xia Zhou and En-Tao Sun

College of Chemistry and Molecular Engineering, Qingdao University of Science and Technology, Qingdao 266042, People's Republic of China

Correspondence e-mail: wenlirong@126.com

Received 12 October 2006
Accepted 30 October 2006

Key indicators

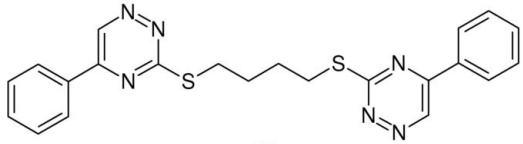
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.125
Data-to-parameter ratio = 15.8

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

In the title compound, $C_{22}H_{20}N_6S_2$, the molecule lies on a centre of inversion and the triazine ring makes a dihedral angle of 8.47 (2)° with the benzene ring.

Comment

1,2,4-Triazine derivatives possess a broad spectrum of biological activity (Said, 2003) and play an important role in the syntheses of heterocyclic compounds (Taylor *et al.*, 1987). In the course of our systematic studies aimed at the synthesis of new symmetrical 1,2,4-triazine compounds, the title compound, (I), was obtained.



(I)

The molecule of (I) (Fig. 1) lies on a centre of inversion. The triazine ring is essentially planar, the largest deviation from the mean plane being 0.032 (2) Å for atom C9. The dihedral angle between the triazine ring and the benzene ring is 8.47 (2)°. Bond distances and angles of the triazine ring are as expected for this type of compound (Wen *et al.*, 2006).

Experimental

1,4-Dibromobutane (0.432 g, 2 mmol) was added to a solution of 5-phenyl-1,2,4-triazine-3-thiol (0.756 g, 4 mmol), KOH (0.224 g, 4 mmol) and tetraethylammonium bromide (0.05 g) in aqueous ethanol (10 ml, 50%). The reaction mixture was refluxed for 6 h, then poured into water (100 ml). The resulting precipitate was collected and recrystallized from EtOH/THF (5:1) to give (I). Single crystals suitable for X-ray analysis were obtained as colourless blocks by slow evaporation of a solution in EtOH/THF (5:1).

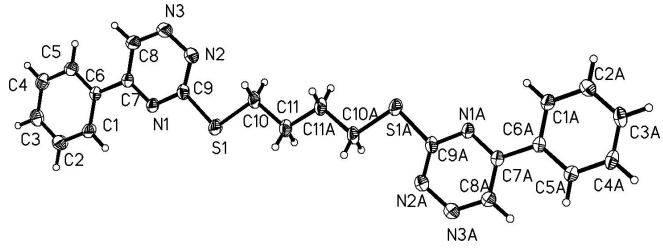


Figure 1
Molecular structure of (I) showing displacement ellipsoids at the 35% probability level. H atoms are shown as spheres of arbitrary radii. Suffix A denotes atoms related by the symmetry operator $(1-x, 1-y, 1-z)$.

Crystal data

$C_{22}H_{20}N_6S_2$
M_r = 432.56
Monoclinic, $P2_1/c$
a = 10.323 (5) Å
b = 11.434 (6) Å
c = 9.562 (5) Å
β = 113.553 (8)°
V = 1034.6 (9) Å^3
Z = 2
D_x = 1.389 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 294 (2) K
Block, colourless
0.32 × 0.16 × 0.08 mm

Data collection

Bruker APEX-II CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.916, T_{max} = 0.978
5764 measured reflections
2153 independent reflections
1434 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 26.6°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.126
S = 1.03
2153 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 0.2027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

H atoms were placed in calculated positions with C—H = 0.93 or 0.97 Å and allowed to ride during subsequent refinement with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

This project was supported by the National Natural Science Foundation of China (20572057).

References

Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Said, M. M. (2003). *Egypt. J. Biomed. Sci.* **11**, 46–59.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Taylor, E. C., Macor, J. E. & Pont, J. L. (1987). *Tetrahedron*, **43**, 5145–5158.
Wen, L. R., Wang, X., Li, M. & Zhai, L. N. (2006). *Chin. J. Struct. Chem.* **25**, 485–490.