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5-Phenyl-3-[3-(5-phenyl-1,2,4-triazin-3-ylsulfanyl)-propylsulfanyl]-1,2,4-triazine

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Key indicators

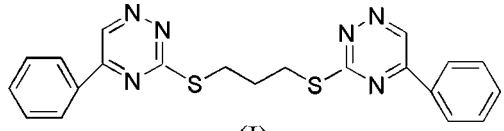
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.126
Data-to-parameter ratio = 15.3

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

The title compound, $C_{21}H_{18}N_6S_2$, crystallizes with one half-molecule in the asymmetric unit; a twofold rotation axis passes through the central C atom. The triazine ring makes a dihedral angle of 10.65 (2)° with the benzene ring.

Comment

1,2,4-Triazine derivatives are an important class of compounds that exhibit various biological activities (Konno *et al.*, 1995) and pharmacological properties (Monge *et al.*,1991). We synthesized the title compound, (I), as part of our systematic studies aimed at developing new bioactive compounds.



(I)

The structure has one half-molecule in the asymmetric unit with the molecule sitting on a twofold axis passing through atom C11 (Fig. 1). All atoms in the triazine ring are essentially coplanar; the largest deviation from the mean plane is 0.031 (2) Å for atom C9. The dihedral angle between the triazine ring and the benzene ring is 10.65 (2)°. Bond distances and angles (Table 1) of the triazine ring are as expected for this type of compound (Wen *et al.*, 2006). The molecules pack in staggered layers stabilized mainly by van der Waals forces.

Experimental

1,4-Dibromopropane (0.404 g, 2 mmol) was added to a solution of 5-phenyl-1,2,4-triazine-3-thiol (0.756 g, 4 mmol) in aqueous ethanol (10 ml, 50%) containing KOH (0.224 g, 4 mmol) and tetraethylammonium bromide (0.05 g). The reaction mixture was refluxed for 6 h and then poured into water (100 ml). The resulting precipitate was collected and crystallized from mixed solvents, hexanes and ethyl acetate (2:1), to give the title compound. Single crystals suitable for X-ray analysis were obtained as colorless blocks by slow evaporation from ethyl acetate (m.p. >503 K, decomposition).

Crystal data

$C_{21}H_{18}N_6S_2$
M_r = 418.53
Monoclinic, $C2/c$
a = 18.204 (8) Å
b = 11.495 (5) Å
c = 9.692 (5) Å
β = 102.483 (8)°
V = 1980.2 (16) Å^3
Z = 4
D_x = 1.404 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 294 (2) K
Block, colorless
0.22 × 0.12 × 0.10 mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.939, T_{max} = 0.972
5456 measured reflections
2014 independent reflections
1231 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 26.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.126
S = 0.95
2014 reflections
132 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.059P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C9	1.745 (2)	N3—C7	1.321 (3)
S1—C10	1.805 (2)	N3—C9	1.347 (3)
N1—C9	1.319 (3)	C7—C8	1.399 (3)
N1—N2	1.350 (3)	C11—C10^{i}	1.517 (3)
N2—C8	1.313 (3)		
C9—S1—C10	103.16 (12)	N2—C8—C7	122.7 (2)
C9—N1—N2	116.81 (18)	N1—C9—N3	127.3 (2)
C7—N3—C9	115.3 (2)	C10^{i}—C11—C10	111.0 (3)
N3—C7—C8	118.9 (2)		

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) set at 1.2U_{eq}(C) for all H atoms.

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*.

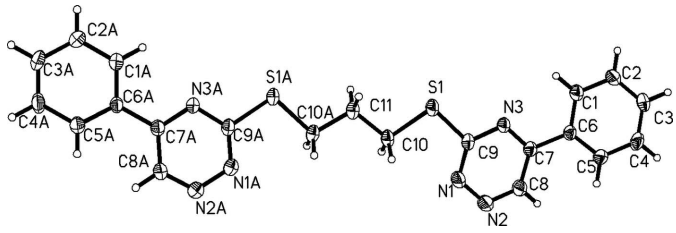


Figure 1
The molecular structure, with displacement parameters at the 35% probability level. The suffix A corresponds to symmetry code i in Table 1.

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