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## Key indicators

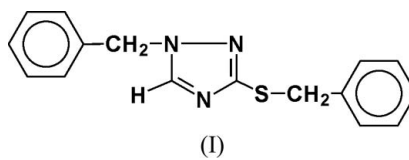
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.043  
 $wR$  factor = 0.125  
Data-to-parameter ratio = 11.9For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.1-Benzyl-3-(benzylsulfanyl)-1*H*-1,2,4-triazole

In the title compound,  $\text{C}_{16}\text{H}_{15}\text{N}_3\text{S}$ , the phenyl rings make dihedral angles of  $73.0$  (1) and  $87.9$  (1) $^\circ$  with the triazole ring. The molecular and crystal structures are stabilized by two intramolecular hydrogen bonds ( $\text{C}-\text{H}\cdots\text{S}$  and  $\text{C}-\text{H}\cdots\text{N}$ ) and one intermolecular  $\text{C}-\text{H}\cdots\text{N}$  hydrogen bond. The latter links molecules into infinite chains.

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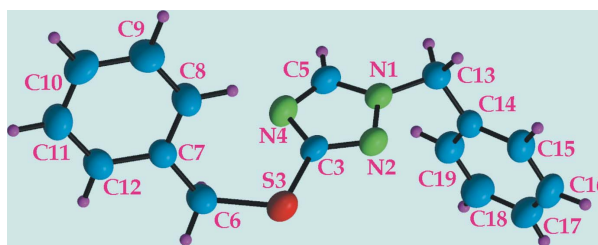
## Comment

1,4-Unsubstituted 1,2,4-triazoles are structurally labile compounds capable of existing in at least three tautomeric forms, *viz.* 1*H*, 2*H* and 4*H*. The present study was intended to provide information on the influence of the tautomeric form on the site of alkylation of the triazole.

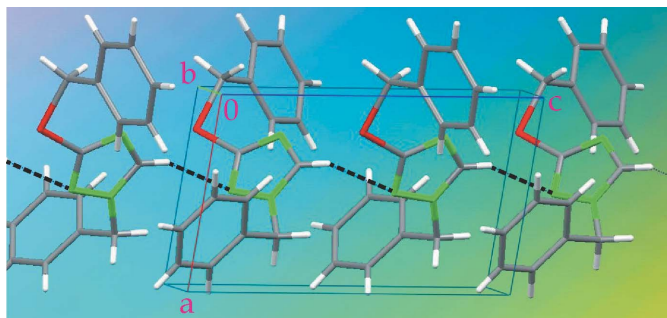


In the title compound, (I), atoms S3, C6 and C13 deviate from the plane of the triazole ring by 0.011 (1), 0.079 (2) and 0.053 (2) Å, respectively. The phenyl substituents C7–C12 and C14–C19 form dihedral angles of  $73.0$  (1) and  $87.9$  (1) $^\circ$ , respectively, with the plane of the triazole ring (Fig. 1). The bond lengths and angles of the triazole ring are similar to those in other 1,3-substituted analogues (Cambridge Structural Database, Version 5.27; Allen, 2002) (Table 1).

Intermolecular  $\text{C}-\text{H}\cdots\text{N}$  interactions are present in the crystal structure (Table 2 and Fig. 2). These contacts link neighbouring molecules into hydrogen-bonded chains along the  $c$  axis. Analysis of the packing in the crystal structure of (I) reveals that there is no accessible volume for solvent inclusion; the packing coefficient is 69.1%. Two intramolecular contacts,  $\text{C}-\text{H}\cdots\text{S}$  and  $\text{C}-\text{H}\cdots\text{N}$ , are present, each resulting in a five-membered ring.



**Figure 1**  
View of the molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.



**Figure 2**  
The molecular packing of (I), viewed approximately along the *b* axis. Black dashed lines indicate the hydrogen-bonding interactions.

## Experimental

The title compound was prepared according to the procedure of Beyer *et al.* (1960) by exhaustive benzylation of 3(5)-mercapto-1,2,4-triazole [3(5) indicates the uncertainty of the tautomeric form of the starting material]. The title compound, (I), was successfully crystallized from acetonitrile. Crystallization from acetone produced crystals having the same unit-cell parameters.

### Crystal data

$C_{16}H_{15}N_3S$   
 $M_r = 281.37$   
Monoclinic,  $P2_1/c$   
 $a = 5.9390$  (8) Å  
 $b = 25.276$  (5) Å  
 $c = 9.567$  (2) Å  
 $\beta = 99.12$  (1)°  
 $V = 1418.0$  (5) Å<sup>3</sup>

$Z = 4$   
 $D_x = 1.318$  Mg m<sup>-3</sup>  
Cu  $K\alpha$  radiation  
 $\mu = 1.96$  mm<sup>-1</sup>  
 $T = 293$  (2) K  
Prism, colourless  
 $0.20 \times 0.10 \times 0.07$  mm

### Data collection

Enraf–Nonius CAD-4  
diffractometer  
 $\omega/2\theta$  scans  
Absorption correction:  $\psi$  scan  
(*CAD-4 Software*; Enraf–Nonius, 1989)  
 $T_{\min} = 0.780$ ,  $T_{\max} = 0.992$   
(expected range = 0.686–0.872)

3166 measured reflections  
2890 independent reflections  
2232 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.032$   
 $\theta_{\text{max}} = 74.2^\circ$   
3 standard reflections  
every 200 reflections  
intensity decay: none

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.043$   
 $wR(F^2) = 0.125$   
 $S = 1.02$   
2890 reflections  
242 parameters  
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0712P)^2 + 0.3185P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.27$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.28$  e Å<sup>-3</sup>  
Extinction correction: *SHELXL97*  
Extinction coefficient: 0.0046 (6)

**Table 1**

Selected geometric parameters (Å, °).

|           |             |            |           |
|-----------|-------------|------------|-----------|
| S3–C3     | 1.7509 (18) | N1–C13     | 1.469 (3) |
| S3–C6     | 1.809 (3)   | N2–C3      | 1.324 (3) |
| N1–N2     | 1.367 (2)   | N4–C3      | 1.351 (2) |
| N1–C5     | 1.320 (3)   | N4–C5      | 1.320 (3) |
| C3–S3–C6  | 102.0 (1)   | S3–C3–N2   | 119.0 (1) |
| N2–N1–C5  | 109.6 (2)   | S3–C3–N4   | 125.8 (1) |
| N2–N1–C13 | 120.7 (2)   | N2–C3–N4   | 115.2 (2) |
| C5–N1–C13 | 129.7 (2)   | N1–C5–N4   | 111.3 (2) |
| N1–N2–C3  | 101.7 (2)   | S3–C6–C7   | 117.2 (2) |
| C3–N4–C5  | 102.2 (2)   | N1–C13–C14 | 111.0 (2) |

**Table 2**

Hydrogen-bond geometry (Å, °).

| <i>D</i> –H... <i>A</i> | <i>D</i> –H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> –H... <i>A</i> |
|-------------------------|-------------|---------------|-----------------------|-------------------------|
| C5–H5...N2 <sup>i</sup> | 0.91 (3)    | 2.57 (3)      | 3.424 (3)             | 155 (2)                 |
| C8–H8...S3              | 0.98 (3)    | 2.83 (3)      | 3.200 (3)             | 103 (2)                 |
| C6–H62...N4             | 0.98 (2)    | 2.55 (3)      | 2.994 (3)             | 107 (2)                 |

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

All H atoms were initially located in a difference Fourier map and refined isotropically; C–H = 0.91 (3)–1.02 (2) Å.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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