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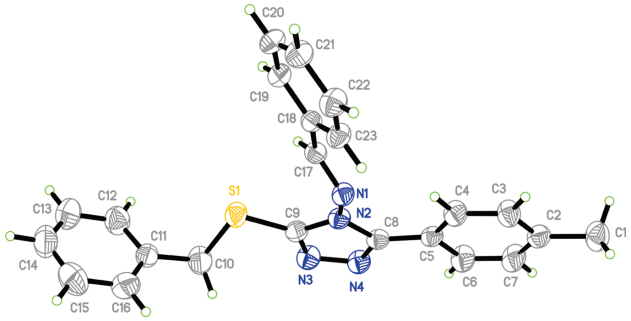
(*E*)-*N*-benzylidene-3-(benzylthio)-5-*p*-tolyl-4*H*-1,2,4-triazol-4-amine, $C_{23}H_{20}N_4S$



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Abstract

$C_{23}H_{20}N_4S$, Monoclinic, $P2_1/n$ (no. 14), $a = 11.439(3)$ Å, $b = 8.868(2)$ Å, $c = 20.557(5)$ Å, $\beta = 104.542(4)°$, $V = 2018.7(8)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0449$, $wR_{ref}(F^2) = 0.1266$, $T = 298(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

The title compound was prepared by the reaction of (*E*)-4-(benzylideneamino)-3-*p*-tolyl-1*H*-1,2,4-triazole-5(4*H*)-thione (2 mmol) and (bromomethyl)benzene (2 mmol) in the mixture of ethanol (40 mL) and triethylamine (1 mL). The mixture was stirred at room temperature for 10 min and the product was obtained by filtration, drying and recrystallization from ethanol. Crystals suitable for X-ray data collection were obtained by slow evaporation of a ethanol

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Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	0.36 × 0.32 × 0.23 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.18 mm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω-scans
$2\theta_{max}$, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9888, 3556, 0.038
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2470
$N(param)_{refined}$:	254
Programs:	Bruker programs [1], SHELX [2]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
S1	0.39452(6)	0.19481(7)	1.06911(3)	0.0731(2)
N1	0.25824(15)	0.0537(2)	0.92820(8)	0.0571(5)
N2	0.36849(15)	0.12915(18)	0.93655(8)	0.0541(4)
N3	0.52124(16)	0.2780(2)	0.97885(9)	0.0674(5)
N4	0.51494(16)	0.2532(2)	0.91147(9)	0.0658(5)
C1	0.2988(2)	−0.0072(3)	0.60699(12)	0.0889(8)
H1A	0.3574	0.0344	0.5858	0.133*
H1B	0.2203	0.0316	0.5855	0.133*
H1C	0.2984	−0.1150	0.6030	0.133*
C2	0.3308(2)	0.0362(3)	0.68024(11)	0.0653(6)
C3	0.2611(2)	−0.0092(3)	0.72176(12)	0.0723(7)
H3A	0.1928	−0.0674	0.7043	0.087*
C4	0.2892(2)	0.0290(3)	0.78859(12)	0.0699(6)
H4A	0.2401	−0.0046	0.8154	0.084*
C5	0.38836(18)	0.1159(2)	0.81662(10)	0.0550(5)
C6	0.4582(2)	0.1619(3)	0.77435(13)	0.0774(7)
H6A	0.5260	0.2214	0.7913	0.093*
C7	0.4294(2)	0.1216(3)	0.70820(13)	0.0827(8)
H7A	0.4789	0.1536	0.6813	0.099*
C8	0.42279(18)	0.1655(2)	0.88644(10)	0.0542(5)
C9	0.43295(19)	0.2019(2)	0.99276(11)	0.0573(5)
C10	0.4673(3)	0.3600(3)	1.11014(13)	0.0893(8)
H10A	0.5544	0.3476	1.1216	0.107*
H10B	0.4464	0.4473	1.0811	0.107*
C11	0.4237(2)	0.3792(3)	1.17174(12)	0.0679(6)
C12	0.4786(3)	0.3052(3)	1.22924(14)	0.0918(8)
H12A	0.5454	0.2450	1.2299	0.110*
C13	0.4384(4)	0.3169(4)	1.28539(16)	0.1119(11)
H13A	0.4783	0.2654	1.3240	0.134*
C14	0.3431(4)	0.4004(4)	1.28632(17)	0.1066(10)
H14A	0.3162	0.4062	1.3253	0.128*
C15	0.2842(3)	0.4778(4)	1.2307(2)	0.1121(11)
H15A	0.2173	0.5369	1.2312	0.134*

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C16	0.3261(3)	0.4670(3)	1.17264(16)	0.0969(9)
H16A	0.2872	0.5200	1.1343	0.116*
C17	0.25665(19)	−0.0428(2)	0.97358(11)	0.0548(5)
H17A	0.3272	−0.0611	1.0067	0.066*
C18	0.14831(19)	−0.1250(2)	0.97532(10)	0.0525(5)
C19	0.1537(2)	−0.2272(2)	1.02667(11)	0.0631(6)
H19A	0.2262	−0.2427	1.0586	0.076*
C20	0.0524(2)	−0.3060(3)	1.03067(12)	0.0712(7)
H20A	0.0562	−0.3740	1.0656	0.085*
C21	−0.0535(2)	−0.2844(3)	0.98356(12)	0.0718(7)
H21A	−0.1220	−0.3380	0.9863	0.086*
C22	−0.0595(2)	−0.1838(3)	0.93209(12)	0.0711(6)
H22A	−0.1320	−0.1696	0.9000	0.085*
C23	0.0407(2)	−0.1045(2)	0.92790(11)	0.0612(6)
H23A	0.0362	−0.0365	0.8929	0.073*

solution after 10 days. (*E*)-4-(benzylideneamino)-3-*p*-tolyl-1*H*-1,2,4-triazole-5(4*H*)-thione was synthesized by the reaction of 4-amino-3-*p*-tolyl-1*H*-1,2,4-triazole-5(4*H*)-thione (2 mmol) and benzaldehyde (2 mmol) with concentrated hydrochloric acid (1 mL) in ethanol (40 mL) refluxed for 3 h.

Experimental details

All H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of Csp^2–H = 0.93 Å with $U_{iso} = 1.2U_{eq}$ (parent atom), and Csp^3–H = 0.96 or 0.97 Å with $U_{iso} = 1.5U_{eq}$ (parent atom).

Discussion

In recent decades, compounds containing the 1,2,4-triazole group have attracted much interest because of their exhibiting various biological activities [3–7]. Recently, (*E*)-3-substituted-4-arylideneamino-5-arylthiol (or alkylthiol)-4H-1,2,4-triazoles have been reported to possess antioxidant, herbicidal, antifungal antineoplastic, and etc [6].

The bond lengths and angles are in the usual ranges. The triazole ring and the benzene ring (C2—C7) are essentially planar and the dihedral angle between them is 2.93(0.15)°. The phenyl ring C18—C23 and the other two aryl moieties (C2—C7 and C11—C16) form two dihedral angles of about 50°. The two rings C2—C7 and C11—C16 are approaching mutually perpendicular, and the dihedral angle between them is 72.29(0.07)°. Both the S—C and C—N bond lengths are in good agreement with the values observed in related compounds. The short C—N bond lengths of 1.304(3) Å for N3—C9 and 1.307(3) Å for N4—C8, respectively, suggest partially localized double bonds.

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