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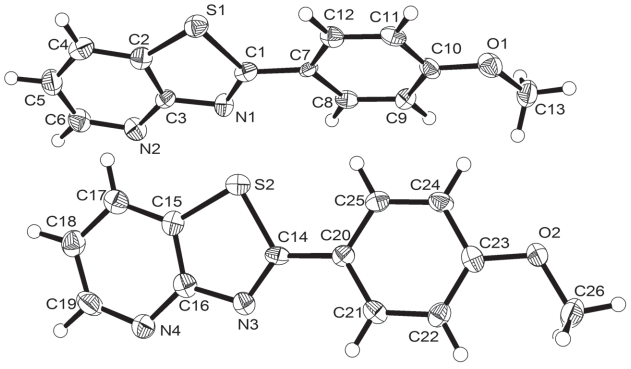
Crystal structure of 2-(4-methoxyphenyl)-1,3-thiazolo[4,5-*b*]pyridine, $C_{13}H_{10}N_2OS$



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Abstract

$C_{13}H_{10}N_2OS$, monoclinic, $P2_1/c$ (no 14), $a = 14.182(3)$ Å, $b = 5.9674(6)$ Å, $c = 26.683(4)$ Å, $\beta = 101.162(17)°$, $V = 2215.4(6)$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0634$, $wR_{ref}(F^2) = 0.1514$, $T = 150$ K.

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

Source of material

2-(4-Methoxyphenyl)-1,3-thiazolo[4,5-*b*]pyridine was obtained in 64% yield from reaction of 4-anisic acid and 3-(diisopropylaminothiocarbonylthio)-2-aminopyridine in

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Table 1: Data collection and handling.

Crystal:	Colourless plate Size 0.42 × 0.11 × 0.03 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	2.7 cm^{-1}
Diffractometer, scan mode:	SuperNova, ω
$2\theta_{max}$, completeness:	59.4°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$	6077, 6077
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3490
$N(param)_{refined}$:	309
Programs:	SHELX [5], CrysAlis [6], WinGX [7]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.6236(3)	0.4406(7)	0.01361(17)	0.0228(10)
C2	0.6729(3)	0.6468(7)	0.09315(16)	0.0253(10)
C3	0.6364(3)	0.4282(7)	0.09712(16)	0.0204(10)
C4	0.7035(3)	0.7725(7)	0.13689(16)	0.0310(10)
H4	0.7271	0.9210	0.1356	0.037*
C5	0.6977(3)	0.6689(8)	0.18229(17)	0.0342(11)
H5	0.7192	0.7468	0.2135	0.041*
C6	0.6614(3)	0.4541(8)	0.18367(16)	0.0307(11)
H6	0.6585	0.3907	0.2160	0.037*
C7	0.6060(3)	0.3708(6)	−0.04020(16)	0.0178(9)
C8	0.5598(3)	0.1690(7)	−0.05484(15)	0.0228(10)
H8	0.5396	0.0786	−0.0296	0.027*
C9	0.5423(3)	0.0955(7)	−0.10473(15)	0.0219(10)
H9	0.5087	−0.0408	−0.1139	0.026*
C10	0.5746(3)	0.2244(7)	−0.14126(15)	0.0244(10)
C11	0.6216(3)	0.4273(7)	−0.12777(16)	0.0244(10)
H11	0.6431	0.5154	−0.1530	0.029*
C12	0.6368(3)	0.4994(7)	−0.07809(15)	0.0245(10)
H12	0.6685	0.6381	−0.0692	0.029*
C13	0.5125(4)	−0.0308(7)	−0.20808(16)	0.0359(12)
H13A	0.5449	−0.1593	−0.1893	0.054*
H13B	0.5095	−0.0523	−0.2448	0.054*
H13C	0.4472	−0.0179	−0.2013	0.054*
C14	0.8828(3)	−0.0573(7)	0.00793(16)	0.0210(9)
C15	0.8865(3)	0.1647(7)	0.08535(15)	0.0240(10)
C16	0.9264(3)	−0.0497(8)	0.09164(17)	0.0258(10)
C17	0.8857(3)	0.2996(8)	0.12715(15)	0.0284(10)
H17	0.8584	0.4454	0.1235	0.034*
C18	0.9263(3)	0.2147(8)	0.17452(16)	0.0317(10)
H18	0.9288	0.3016	0.2046	0.038*

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
C19	0.9631(3)	−0.0009(8)	0.17702(18)	0.0375(12)
H19	0.9890	−0.0578	0.2101	0.045*
C20	0.8632(3)	−0.1351(7)	−0.04439(16)	0.0216(10)
C21	0.9034(3)	−0.3353(7)	−0.05740(15)	0.0228(10)
H21	0.9439	−0.4184	−0.0314	0.027*
C22	0.8863(3)	−0.4163(7)	−0.10669(16)	0.0252(10)
H22	0.9145	−0.5530	−0.1146	0.030*
C23	0.8270(3)	−0.2945(8)	−0.14471(16)	0.0249(10)
C24	0.7868(3)	−0.0925(7)	−0.13265(16)	0.0258(10)
H24	0.7465	−0.0087	−0.1586	0.031*
C25	0.8057(3)	−0.0157(7)	−0.08326(15)	0.0246(10)
H25	0.7788	0.1228	−0.0755	0.030*
C26	0.8395(4)	−0.5675(8)	−0.20821(17)	0.0379(12)
H26A	0.9099	−0.5647	−0.2010	0.057*
H26B	0.8162	−0.5964	−0.2447	0.057*
H26C	0.8169	−0.6863	−0.1881	0.057*
N1	0.6086(2)	0.3174(6)	0.05099(13)	0.0236(8)
N2	0.6299(3)	0.3306(6)	0.14154(13)	0.0289(9)
N3	0.9245(2)	−0.1732(6)	0.04762(13)	0.0239(8)
N4	0.9657(3)	−0.1362(6)	0.13766(14)	0.0335(10)
O1	0.5651(2)	0.1696(5)	−0.19173(10)	0.0309(7)
O2	0.8038(2)	−0.3560(5)	−0.19494(10)	0.0298(7)
S1	0.67055(8)	0.7093(2)	0.03003(4)	0.0279(3)
S2	0.84480(8)	0.2144(2)	0.02155(4)	0.0270(3)

phosphorus oxychloride under reflux for 4 h [1] or in 82% yield from treatment of 3-(diisopropylaminothiocarbonylthio)-2-(4-methoybenzoylamino)pyridine with hydrochloric acid under reflux for 5 h [2]. Colourless crystals of the title compound were obtained *via* crystallization from diethyl ether.

Experimental details

The crystal was twinned and refinement was performed using the option HKLF 5 in SHELX [5]. H atoms were placed in calculated positions and refined using a riding model, with U_{iso}(H) set to 1.2U_{eq}(C) and aromatic C—H distance of 0.93 Å. The methyl (C—H = 0.96 Å) groups were allowed to rotate around the C—C bond (HFIX 137 option in SHELX [5]) with U_{iso}(H) set to 1.5U_{eq}(C).

Discussion

Various thiazolopyridines have been synthesised *via* various synthetic methods and many derivatives have shown interesting biological applications [3, 4]. The asymmetric unit of the crystal structure of the title compound consists of two independent molecules of $C_{13}H_{10}N_2OS$. The methoxyphenyl groups in both molecules are planar, as illustrated by C_{Me}-O-C_{Ph}-C_{Ph}torsion angles of 3.8(5)° and 3.4(6)°. The dihedral angles between the planes through the methoxyphenyl and thiazolopyridine groups of the two molecules are 9.6(2)° and 10.0(1)°, indicating that both molecules are nearly planar. In the crystal, π-π interaction occurs between inversion-related molecules separated by a distance of 3.4 Å of the corresponding planes.

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