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Crystal structure of 2-(bromomethyl)-4-(4-chlorophenyl)-1-tosylpyrrolidine, $C_{18}H_{19}BrClNO_2S_2$

Table 1: Data collection and handling.

Crystal:	Colourless blocks
Wavelength:	Size $0.36 \times 0.28 \times 0.14$ mm
μ :	Mo K_{α} radiation (0.71073 Å)
Diffractometer, scan mode:	24.7 cm^{-1}
$2\theta_{\text{max}}$, completeness:	Bruker APEX-II, φ and ω
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	50.2°, >99%
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	8828, 3294, 0.046
$N(\text{param})_{\text{refined}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1991
Programs:	218
	SHELX [12], Bruker programs [13]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.29445(3)	0.60745(12)	0.44266(4)	0.0902(3)
Cl1	0.55481(7)	0.1519(3)	0.93250(10)	0.0947(5)
S1	0.16851(6)	0.6687(2)	0.63876(10)	0.0631(4)
N1	0.23440(16)	0.5427(7)	0.6284(2)	0.0511(10)
O1	0.18312(17)	0.8940(5)	0.6708(3)	0.0904(13)
O2	0.13075(16)	0.6354(7)	0.5553(2)	0.0915(13)
C1	0.0315(3)	0.2131(12)	0.9264(4)	0.094(2)
H1A	0.0465	0.2733	0.9842	0.140*
H1B	0.0380	0.0510	0.9260	0.140*
H1C	−0.0126	0.2454	0.9142	0.140*
C2	0.0672(2)	0.3227(9)	0.8550(3)	0.0568(13)
C3	0.1022(2)	0.5152(11)	0.8729(3)	0.0733(16)
H3	0.1048	0.5764	0.9304	0.088*
C4	0.1337(2)	0.6219(9)	0.8084(4)	0.0661(14)
H4	0.1570	0.7535	0.8223	0.079*
C5	0.13026(19)	0.5312(7)	0.7232(3)	0.0455(11)
C6	0.0962(2)	0.3362(8)	0.7041(3)	0.0519(12)
H6	0.0940	0.2730	0.6469	0.062*
C7	0.0650(2)	0.2336(8)	0.7700(3)	0.0566(13)
H7	0.0419	0.1012	0.7566	0.068*
C8	0.2836(2)	0.5450(8)	0.7046(3)	0.0573(13)
H8A	0.2666	0.5954	0.7591	0.069*
H8B	0.3181	0.6449	0.6925	0.069*
C9	0.3054(2)	0.2989(7)	0.7128(3)	0.0499(11)
H9	0.2740	0.2137	0.7431	0.060*
C10	0.2997(2)	0.2250(8)	0.6152(3)	0.0542(12)
H10A	0.3354	0.2783	0.5856	0.065*
H10B	0.2974	0.0601	0.6104	0.065*
C11	0.2393(2)	0.3334(8)	0.5739(3)	0.0554(12)
H11	0.2044	0.2325	0.5856	0.066*

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Abstract

$C_{18}H_{19}BrClNO_2S_2$, monoclinic, $P2_1/c$ (no. 14), $a = 21.324(6)$ Å, $b = 5.8597(16)$ Å, $c = 14.966(4)$ Å, $\beta = 95.558(5)^\circ$, $V = 1861.2(9)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0454$, $wR_{\text{ref}}(F^2) = 0.1258$, $T = 296(2)$ K.

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The asymmetric unit of the 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.

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Table 2 (continued)

Atom	x	y	z	U_{iso}^*/U_{eq}
C12	0.2351(3)	0.3768(9)	0.4738(3)	0.0737(16)
H12A	0.1927	0.4257	0.4532	0.088*
H12B	0.2433	0.2357	0.4432	0.088*
C13	0.3686(2)	0.2659(8)	0.7663(3)	0.0513(12)
C14	0.4063(2)	0.0825(8)	0.7529(4)	0.0666(14)
H14	0.3934	−0.0204	0.7075	0.080*
C15	0.4627(2)	0.0444(9)	0.8044(4)	0.0679(15)
H15	0.4869	−0.0832	0.7943	0.082*
C16	0.4821(2)	0.1958(10)	0.8698(3)	0.0665(14)
C17	0.4470(3)	0.3828(11)	0.8847(4)	0.099(2)
H17	0.4608	0.4870	0.9292	0.118*
C18	0.3907(3)	0.4164(10)	0.8331(4)	0.0837(19)
H18	0.3667	0.5444	0.8437	0.100*

Source of material

The mixture of *N*-(2-(4-chlorophenyl)pent-4-en-1-yl)-4-methylbenzenesulfonamide, K₂CO₃, bis(triphenylphosphine) palladium(II) dichloride and *N*-bromosuccinimide was stirred for 1 h at room temperature to obtain the title compound with the yield of 94%. The solution of *n*-heptane and ethyl acetate was left to gradually volatilize in the atmosphere to obtain the single crystal.

Experimental details

The U_{iso} values of the hydrogen atoms of methyl groups were set to 1.5 U_{eq} (C) and the U_{iso} values of phenyl and methylene hydrogen atoms were set to 1.2 U_{eq} (C).

Discussion

The title compound is an important building block for the synthesis of bioactive molecules. The bromine atom can easily be replaced by other functional groups to generate corresponding products [1–7]. They have been widely used as broad-spectrum anti-bacterial agents [8], these been reported in the utilize of anti-cancer research [9, 10] and also arouse a significant pharmacological interest [11]. In the title structure, the pyrrolidine ring adapts a twisted envelope conformation. The dihedral angle between the two phenyl ring systems is 87.68(3)°, and the dihedral angle between the mean plane of sulfonyl group (O1, S1 and O2) and its connected phenyl ring is 55.90(6)°, but the dihedral angle with the other phenyl ring is 37.69(3)°. No conventional hydrogen bonds were found.

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