Crystal structure of 6-azido-1,4-bis(tosyl)-1,4-diazepane—DMSO (1:1), $C_{19}H_{23}N_5O_4S_2 \cdot C_2H_6OS$

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Table 3. Atomic coordinates and displacement parameters (in Å²).

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
S(1)	4a	0.6238(1)	0.28744(5)	0.0806(1)	0.0424(6)	0.0398(6)	0.0466(7)	0.0028(5)	0.0136(5)	0.0069(5)
S(2)	4a	0.7341(1)	0.05420(5)	0.2894(1)	0.0450(7)	0.0444(7)	0.0493(7)	0.0026(5)	0.0173(5)	−0.0007(6)
C(1)	4a	0.6481(5)	0.1299(2)	−0.0523(5)	0.078(4)	0.049(3)	0.030(3)	−0.003(3)	0.013(3)	−0.012(2)
C(2)	4a	0.7250(5)	0.0833(2)	0.0424(5)	0.067(3)	0.039(3)	0.052(3)	0.003(2)	0.020(3)	−0.008(2)
N(2)	4a	0.7493(3)	0.1022(2)	0.1798(4)	0.041(2)	0.034(2)	0.046(2)	−0.000(2)	0.004(2)	−0.000(2)
C(3)	4a	0.8444(5)	0.1494(2)	0.2212(6)	0.043(3)	0.042(3)	0.061(3)	−0.003(2)	−0.003(2)	0.005(2)
C(4)	4a	0.7984(5)	0.2127(2)	0.2080(6)	0.046(3)	0.045(3)	0.054(3)	−0.002(2)	−0.005(2)	0.008(2)
N(3)	4a	0.6948(3)	0.2220(2)	0.0887(4)	0.045(2)	0.031(2)	0.034(2)	−0.002(2)	0.004(2)	0.000(2)
C(5)	4a	0.6993(6)	0.1956(2)	−0.0348(5)	0.074(4)	0.047(3)	0.048(3)	0.002(3)	0.025(3)	0.006(2)
N(11)	4a	0.5225(5)	0.1279(2)	−0.0577(5)	0.064(3)	0.065(3)	0.048(3)	−0.014(2)	−0.006(2)	−0.008(2)
N(12)	4a	0.4958(4)	0.1382(2)	0.0449(6)	0.039(3)	0.059(3)	0.066(3)	−0.010(2)	−0.004(2)	−0.003(2)
N(13)	4a	1.4560(5)	−0.1456(3)	0.6268(7)	0.047(3)	0.114(5)	0.088(4)	0.013(3)	0.021(3)	0.013(4)
O(21)	4a	0.7292(4)	0.0899(2)	0.4009(4)	0.070(2)	0.068(2)	0.062(2)	0.017(2)	0.029(2)	−0.003(2)
O(22)	4a	0.6375(3)	0.0143(2)	0.2270(4)	0.053(2)	0.057(2)	0.082(3)	−0.009(2)	0.024(2)	0.005(2)
C(21)	4a	0.8675(4)	0.0106(2)	0.3419(5)	0.053(3)	0.037(3)	0.037(2)	0.002(2)	0.016(2)	0.003(2)
C(22)	4a	0.9599(5)	0.0285(2)	0.4514(5)	0.064(3)	0.044(3)	0.050(3)	0.003(3)	0.015(3)	0.001(2)
C(23)	4a	1.0637(5)	−0.0054(3)	0.4896(6)	0.061(3)	0.056(3)	0.053(3)	0.006(3)	0.006(3)	0.000(3)
C(24)	4a	1.0774(6)	−0.0564(3)	0.4217(6)	0.068(4)	0.063(4)	0.057(3)	0.024(3)	0.015(3)	0.011(3)
C(25)	4a	0.9833(5)	−0.0749(3)	0.3126(6)	0.074(4)	0.051(3)	0.055(3)	0.019(3)	0.013(3)	−0.006(3)
C(26)	4a	0.8789(5)	−0.0410(2)	0.2716(5)	0.067(4)	0.052(3)	0.040(3)	0.012(3)	0.008(3)	−0.001(2)
C(241)	4a	1.1930(8)	−0.0934(4)	0.4674(8)	0.096(5)	0.115(6)	0.079(5)	0.055(5)	0.002(4)	−0.006(4)
O(11)	4a	0.5122(3)	0.2817(2)	−0.0225(4)	0.040(2)	0.064(2)	0.075(3)	−0.000(2)	0.002(2)	0.021(2)
O(12)	4a	0.6228(4)	0.3014(2)	0.2108(4)	0.082(3)	0.058(2)	0.060(2)	0.006(2)	0.037(2)	0.004(2)
C(11)	4a	0.7108(4)	0.3433(2)	0.0319(5)	0.046(3)	0.034(2)	0.040(3)	0.004(2)	0.009(2)	0.004(2)
C(12)	4a	0.8040(5)	0.3725(2)	0.1249(5)	0.062(3)	0.047(3)	0.043(3)	−0.002(3)	0.007(3)	−0.003(2)
C(13)	4a	0.8727(5)	0.4141(2)	0.0861(6)	0.057(3)	0.053(3)	0.061(3)	−0.013(3)	0.005(3)	−0.009(3)
C(14)	4a	0.8513(5)	0.4283(3)	−0.0473(6)	0.064(4)	0.048(3)	0.077(4)	−0.013(3)	0.031(3)	0.001(3)
C(15)	4a	0.7583(5)	0.3984(2)	−0.1403(5)	0.068(3)	0.055(3)	0.047(3)	−0.007(3)	0.022(3)	0.006(3)
C(16)	4a	0.6876(5)	0.3556(2)	−0.1013(5)	0.051(3)	0.042(3)	0.045(3)	0.003(2)	0.010(2)	0.000(2)
C(141)	4a	0.9304(8)	0.4736(4)	−0.0923(9)	0.104(6)	0.071(4)	0.119(6)	−0.036(4)	0.047(5)	−0.003(4)
S(1L)	4a	0.6054(2)	0.2139(1)	−0.4038(2)	0.095(1)	0.136(2)	0.057(1)	−0.024(1)	0.0272(9)	−0.010(1)
C(1L)	4a	1.5308(7)	−0.2052(3)	0.9293(6)	0.081(5)	0.088(5)	0.063(4)	0.004(4)	0.025(4)	0.011(4)
O(1L)	4a	1.0623(7)	0.2280(4)	0.1368(8)	0.122(5)	0.205(8)	0.144(6)	0.021(5)	0.060(5)	0.113(6)
C(2L)	4a	0.7508(8)	0.2278(5)	0.5866(9)	0.084(5)	0.129(7)	0.108(7)	−0.012(5)	0.021(5)	−0.033(6)

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