

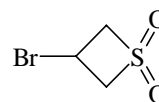
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C₃H₅BrO₂S

3-Bromothietane 1,1-dioxide

C_s

r_g	Å ^{a)}	θ_α	deg ^{a)}
C–H	1.109(7)	C–C–S	89.2(5)
C–C	1.567(6)	C–S–C	80.4(4)
S–C	1.801(4)	C–C–C	95.8(7)
S=O	1.442(3)	O=S=O	121.5(5)
C–Br	1.933(6)	ϕ ^{b)}	25.0(14)



The presence of the equatorial and axial Br positions was indicated, the relative abundance of the former being estimated to be 76(10) % at the nozzle temperature, 453 K. The overall structure of the free molecule, analyzed with identical geometries for both conformers except for the Br positions, is in agreement with that determined in the crystal [1], but the ring is more puckered, the C–C bond is longer and the SO₂ group is more open in the gas phase than were found in the crystal.

^{a)} Estimated total errors.

^{b)} Dihedral angle between the CCC and CSC planes.

Brunvoll, J., Chiang, J.F., Hargittai, I.: Acta Crystallogr., Sect. C **42** (1986) 94.

[1] Chiang, J.F.: Acta Crystallogr., Sect. C **39** (1983) 737.