

1763
MW

C₄H₈S

Allyl methyl sulfide

C₁
H2C=CH-CH2-S-CH3

r_0	Å ^{a)}	θ_0	deg ^{a)}
C(1)=C(2)	1.354 ^{b)}	C(1)=C(2)-C(3)	121.6 ^{b)}
C(2)-C(3)	1.486 ^{b)}	C(2)-C(3)-S	110.9 ^{b)}
S-C(3)	1.819 ^{b)}	C(3)-S-C(4)	102.3(30)
S-C(4)	1.806(30)	H(1)-C(1)=C(2)	121.5 ^{b)}
C(1)-H(1)	1.098 ^{b)}	H(2)-C(1)=C(2)	119.2 ^{b)}
C(1)-H(2)	1.054 ^{b)}	H(3)-C(2)=C(1)	119.0 ^{b)}
C(2)-H(3)	1.090 ^{b)}	H(4)-C(3)-C(2)	107.4 ^{b)}
C(3)-H(4)	1.127 ^{b)}	H(5)-C(3)-C(2)	105.2 ^{b)}
C(3)-H(5)	1.137 ^{b)}	H-C(4)-S	109.5 ^{b)}
C(4)-H	1.095(50)	C(1)=C(2)-C(3)-S ^{c)}	120.0 ^{b)}
		C(1)=C(2)-C(3)-H(5) ^{c)}	120.0 ^{b)}
		C(2)-C(3)-S-C(4) ^{c)}	60.0 ^{b)}

The sulfur atom is *skew* with respect to the C=C bond, and the methyl group is *gauche* with respect to the C-C bond.

^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

^{c)} Dihedral angle.

Fantoni, A.C.: J. Mol. Struct. **243** (1991) 131.

