

1174
MW

C₃H₄S

2-Propyne-1-thiol
Propargyl mercaptan

C₁ (*gauche*)
HC≡C-CH₂-SH

r_0	Å	θ_0	deg
S-H	1.336 ^{a)}	S-C-C	113.01(1)
C-H (in CH ₂)	1.091 ^{a)}	C-S-H	98(1)
C-C	1.460 ^{a)}	H-C-C	111.5 ^{a)}
C≡C	1.207 ^{a)}	ϕ ^{b)}	124(3)
C-H (in CH)	1.057 ^{a)}		
C-S	1.819 ^{a)}		

^{a)} Assumed.

^{b)} Internal rotation angle measured at the *gauche* conformation and computed starting from the *trans* conformation.

Mirri, A.M., Scappini, F., Cervellati, R., Favero, P.G.: J. Mol. Spectrosc. **63** (1976) 509.
Erratum: J. Mol. Spectrosc. **65** (1977) 336.