

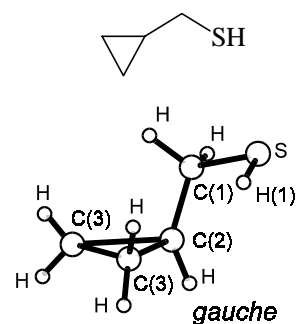
1765 C₄H₈S
MW

Cyclopropanemethanethiol

C₁

r_0	Å	θ_0	deg
C–C(ring)	1.512 ^{a)}	C–C–C(ring)	60.0 ^{a)}
C(1)–C(2)	1.520 ^{a)}	H–C(3)–H	116.0 ^{a)}
C(1)–S	1.814 ^{a)}	H–C(2)–C(1)	116.0 ^{a)}
S–H	1.340 ^{a)}	C(2)–C(1)–H	109.47 ^{a)}
C(1)–H	1.093 ^{a)}	C(1)–S–H	96.5 ^{a)}
C(ring)–H	1.083 ^{a)}	S–C(1)–C(2)–H ^{b)}	60(1)
		H–S–C(1)–C(2) ^{c)}	57(1)

Atom	$ a_s $ [Å]	$ b_s $ [Å]	$ c_s $ [Å]
H(1)	1.4004	1.3326	0.4102
S	1.8735	0.195	0.140



This conformer, which is stabilized by a very weak H bond formed between the H atom in the thiol group and the "quasi- π " electrons of the cyclopropyl ring, is at least 3 kJ mol⁻¹ more stable than any other hypothetical conformation. Structural parameters were kept fixed. The HC(ring)H planes and the HC(2)C(1) plane are perpendicular to the ring.

^{a)} Assumed.

^{b)} Fitted dihedral angle. The H–C(2)–C(1)–H dihedral angles are 60° and 180°.

^{c)} Fitted dihedral angle.

Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand. **45** (1991) 354.