

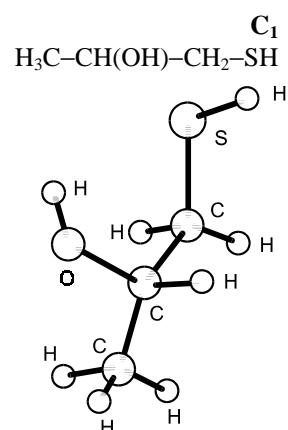
1348
MW

C₃H₈OS

1-Mercapto-2-propanol

r_0	Å
C–S	1.806 ^{a)}
C–O	1.415 ^{a)}
C–C	1.530 ^{a)}
S–H	1.340 ^{a)}
O–H	0.950 ^{a)}
C–H	1.093 ^{a)}

θ_0	deg
C–S–H	96.5 ^{a)}
C–O–H	104.0 ^{a)}
C–C–S	113.5 ^{a)}
C–C–O	112.5 ^{a)}
C–C–C	110.0 ^{a)}
C–C–H	109.47 ^{a)}
C–C–O–H	60.0 ^{a)} ^{b)}
H–S–C–C	60.0 ^{a)} ^{b)}
O–C–C–S	58(2) ^{b)}



One conformer was detected, which is at least 3 kJ mol^{−1} more stable than others.
Dihedral angles around the carbon atoms were assumed to be 120°.

^{a)} Assumed.

^{b)} From *syn* position.

Marstokk, K.-M., Møllendal, H., Samdal, S.: Acta Chem. Scand. **44** (1990) 339.