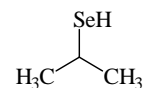


1357  
MW

$\text{C}_3\text{H}_8\text{Se}$

2-Propaneselenol

$\text{C}_s$  (*trans*)  
 $\text{C}_1$  (*gauche*)



$r_0$	$\text{\AA}$		$\theta_0$	deg	
	<i>trans</i>	<i>gauche</i>		<i>trans</i>	<i>gauche</i>
C–H	1.546(3)	1.542(3)	C–C–C	110.9(3)	110.9 <sup>a)</sup>
C–Se	1.930(3)	1.939(3)	Se–C–C( <i>gauche</i> ) <sup>b)</sup>	113.1(2)	113.0(31)
Se–H	1.458(15)	1.446(21)	Se–C–C( <i>trans</i> ) <sup>b)</sup>		108.5(34)
			C–Se–H	93.4(10)	93.7(10)
			$\tau$ <sup>c)</sup>	180 <sup>a)</sup>	16.8(18)

The tetrahedral angles and lengths of 1.091 Å for the C–H bond in the two methyl groups and 1.100 Å for the C–H bond connecting the H atom and the central C atom are assumed. Remaining angles around the central C atom are as follows: for the *trans* conformer H–C–Se = 107.06°, H–C–C = 106.32°; for the *gauche* conformer: H–C–Se = 109.4°, H–C–C(*gauche*) = 107.05° and H–C–C(*trans*) = 107.85°.

<sup>a)</sup> Assumed.

<sup>b)</sup> The C atom in the methyl group lies in the *gauche* and *trans* positions, respectively, with respect to the H atom in the selenol group.

<sup>c)</sup> Dihedral angle H–C–Se–H.

Nakagawa, J., Nagayama, A., Hayashi, M.: J. Mol. Spectrosc. **99** (1983) 415.