

1353
MW

C₃H₈S

1-Propanethiol

C_s (*trans*)
C₁ (*gauche*)
H₃C–CH₂–CH₂–SH

<i>r_s</i>	Å ^{a)}		<i>θ_s</i>	deg ^{a)}	
	<i>gauche</i>	<i>trans</i>		<i>gauche</i>	<i>trans</i>
C(3)–C(2)	1.536(20)	1.536 ^{b)}	H–C(3)–H	108.0 ^{b)}	108.0 ^{b)}
C(3)–H	1.094 ^{b)}	1.094 ^{b)}	H–C(3)–C(2)	111.0 ^{b)}	111.0 ^{b)}
C(1)–C(2)	1.528(10)	1.529(10)	C–C–C	111.7(20)	111.7 ^{b)}
C(2)–H	1.091(15)	1.092(15)	C(3)–C(2)–H	108.4(20) ^{d)}	107.9(20) ^{d)}
C(1)–S	1.814(10)	1.820(10)	H–C(2)–C(1)	110.6(20)	110.6(20)
C(1)–H	1.089(15)	1.090(15)	H–C(2)–H	106.9(20)	108.1(20)
S–H	1.336(15)	1.336 ^{b)}	C(2)–C(1)–S	113.6(10)	108.6(10)
			H(1)–C(1)–S ^{c)}	104.9(20)	109.4(20)
			H(2)–C(1)–S ^{c)}	109.3(20)	109.4(20)
			H(1)–C(1)–C(2) ^{c)}	110.7(20)	110.2(20)
			H(2)–C(1)–C(2) ^{c)}	111.3(20)	110.2(20)
			H(1)–C(1)–H(2)	106.6(20)	108.9(20)
			C(1)–S–H	96.0(20)	96.2(20)
			<i>τ</i> ^{e)}	61.8(20)	180

The conformation about C(1)–(2) is *trans* for both forms.
Energy difference $\Delta E(\text{trans} - \text{gauche})$ is 136(40) cm^{−1}.

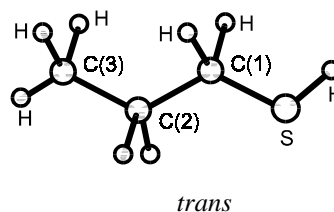
^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

^{c)} The symbols H(1) and H(2) denote the hydrogen atoms which are located on the same and opposite directions, respectively, to the hydrogen atom of the thiol group with respect to the CCCS plane.

^{d)} Calculated from $\theta(\text{C} - \text{C} - \text{C})$, $\theta(\text{H} - \text{C} - \text{CH}_2)$ and $\theta(\text{H} - \text{C} - \text{H})$.

^{e)} Dihedral angle C–C–S–H.



Nakagawa, J., Hayashi, M.: J. Mol. Spectrosc. **85** (1981) 327.