

1354
MW

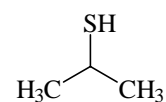
C₃H₈S

2-Propanethiol
Isopropyl mercaptan

C_s (*trans*)
C₁ (*gauche*)

<i>trans</i>			
<i>r</i> ₀	Å ^{a)}	<i>θ</i> ₀	deg ^{a)}
C–S	1.849(2)	C–C–C	113.6(2)
S–H	1.345(2)	C–C–S	111.2(2)
C–C	1.520 ^{a)}	C–S–H	96.5(5)
C–H	1.091 ^{a)}	H–C–C	109.5 ^{a)}

Atom (thiol group)	<i>a</i> _s [Å]	<i>b</i> _s [Å]	<i>c</i> _s [Å]
<i>trans</i>			
H	1.1279	0.0	1.3396
S	1.3060	0.0	0.02
<i>gauche</i>			
H	1.5743	1.1739	0.4558



The *trans* form is more stable than the *gauche* form by 57 cal mol^{−1}.

^{a)} Assumed.

Griffiths, J.H., Boggs, J.E.: J. Mol. Spectrosc. **56** (1975) 257.