

1224
MW

C₃H₅NS

3-Mercaptopropionitrile

C₁ (*gauche*)
C₁ (*anti* II)
HS-CH₂-CH₂-C≡N

r_0	Å ^{a)}
C(3)-S	1.820 ^{a)}
C(2)-C(3)	1.530 ^{a)}
C(1)-C(2)	1.474 ^{a)}
C≡N	1.157 ^{a)}
C-H	1.093 ^{a)}

	<i>gauche</i>	<i>anti</i> II
S-H	1.37(10)	1.322 ^{a)}

θ_0	deg ^{a)}
C-C-C	110.5 ^{a)}
C-S-H	96.2 ^{a)}
C-C≡N	180.00 ^{a)}
C-C-H	109.48 ^{a)}
H-C-H	109.48 ^{a)}
τ_1 ^{b)}	120.00 ^{a)}

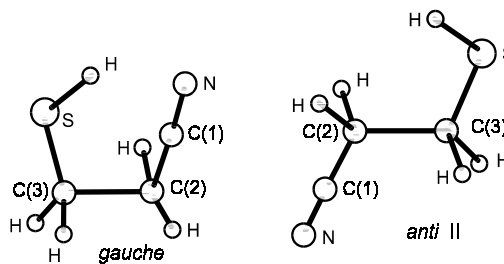
	<i>gauche</i>	<i>anti</i> II
C-C-S	114.0(15)	111.5(10)
τ_2 ^{c)}	65(3)	180.00 ^{a)}

The *gauche* form is more stable than the *anti* II form by 1.3(20) kJ mol⁻¹.

^{a)} Assumed.

^{b)} Dihedral angle H-S-C-C from *anti*.

^{c)} Dihedral angle S-C-C-C from *syn*.



Marstokk, K.-M., Møllendal, H.: Acta Chem. Scand. Ser. A **37** (1983) 477.