

1258
MW

C₃H₆N₂

3-Aminopropionitrile

C₁ (*gauche* I)
C₁ (*gauche* II)
N≡C–CH₂–CH₂–NH₂

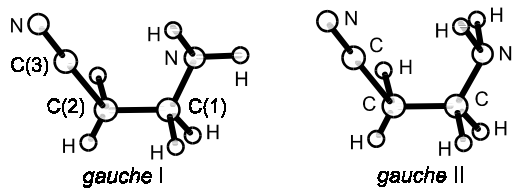
r_0	Å ^{a)}	θ_0	deg ^{a)}
C(3)≡N	1.157 ^{a)}	C(2)–C(3)≡N	180.0 ^{a)}
C(1)–N	1.475 ^{a)}	C–C–H	109.5 ^{a)}
C(2)–C(3)	1.463 ^{a)}	C–N–H	111.0 ^{a)}
C(1)–C(2)	1.548 ^{a)}	C–C–C	110.5 ^{a)}
C–H	1.091 ^{a)}	τ_1 ^{b)}	60 or 180
N–H	1.017 ^{a)}		<i>gauche</i> I <i>gauche</i> II
		N–C(1)–C(2)	108.0(15) 114.0(15)
		τ_2 ^{c)}	63(3) 59(3)

The energy difference between the two forms I and II is 0(2) kJ mol^{–1}.

^{a)} Assumed.

^{b)} Dihedral angle H–N–C–C
from *syn*.

^{c)} Dihedral angle N–C–C–C
from *syn*.



Braathén, O.-A., Marstokk, K.-M., Møllendal, H.: Acta. Chem. Scand. Ser. A **37** (1983) 493.