

1298
ED, MW

C₃H₇Cl

1-Chloropropane
Propyl chloride

C_s (*anti*)
C₁ (*gauche*)
H₃C–CH₂–CH₂Cl

r_g	Å ^{a)}
C–H (average)	1.113(3)
C–C (average)	1.525(2)
C–Cl (average)	1.796(2)

r_z	Å ^{a)}
C–H (average)	1.094(3)
C–C (average)	1.522(2)
C–Cl (average)	1.794(2)

θ_z	deg ^{a)}	
ϕ ^{b)}	129.4(16)	
	<i>gauche</i>	<i>anti</i>
C–C–C	113.9(5)	111.3(13)
C–C–Cl	112.2(6)	111.3(7)
τ ^{c)}	63.9(12)	180

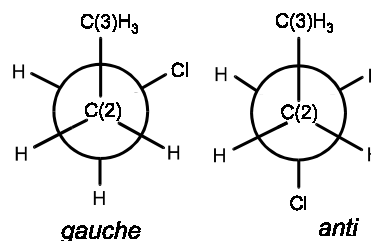
The listed values are weighted averages of the two conformers, *gauche* and *anti*, unless specified. The abundance ratio of the *anti* conformer is found to be 38(3)%. The enthalpy difference is $\Delta H = H(\textit{gauche}) - H(\textit{anti}) = 45(70) \text{ cal mol}^{-1}$.

The measurements were made at room temperature.

^{a)} Estimated limits of error.

^{b)} Angle between the bisector of the H–C(1)–H angle and the C(1)–C(2) bond.

^{c)} Dihedral angle C–C–C–Cl.



Yamanouchi, K., Sugie, M., Takeo, H., Matsumura, C.,
Kuchitsu, K.: J. Phys. Chem. **88** (1984) 2315.