

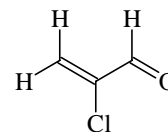
1090
ED

C₃H₃ClO

2-Chloro-2-propenal
2-Chloroacrylaldehyde

C_s (*anti*)
C₁ (*gauche*)

r_g	Å ^{a)}	θ_α	deg ^{a)}
C=O	1.212(3)	C–C=O (<i>anti</i>)	122.8(15)
C–C	1.477(6)	C–C=O (<i>gauche</i>)	121.6(27)
C=C	1.328(6)	C–C–Cl	117.3(7)
C–Cl	1.723(2)	C–C–C	121.1(6)
		H–C–H	117(10)
		τ (<i>gauche</i>) ^{b)}	136(8)



The amount of (*anti*) conformer at 20 °C is 68(5)% and at 150 °C 50(4)%. *anti*

$\Delta E^\circ = E^\circ(\textit{gauche}) - E^\circ(\textit{anti}) = 1.4(5) \text{ kcal mol}^{-1}$,

$\Delta S^\circ = S^\circ(\textit{gauche}) - S^\circ(\textit{anti}) = 2.0(13) \text{ cal mol}^{-1} \text{ K}^{-1}$.

The nozzle temperatures were 20(5) and 150(5) °C.

The parameters for 20(5) °C are listed.

^{a)} Three times the estimated standard errors.

^{b)} C=C–C=O torsion angle; $\tau = 0^\circ$ for *anti* position.

Nippan, M.E., Sadova, N.I., Golubinskii, A.V., Vilkov, L.V.: Zh. Strukt. Khim. **27** No.2 (1986) 47; Russ. J. Struct. Chem. (Engl. Transl.) **27** (1986) 215.