

1801
ED

C₄H₁₀

Butane

C_{2h} (*anti*)
C₂ (*gauche*)
H₃C–CH₂–CH₂–CH₃

r_g	\AA^a	θ_α	deg^a
C–C	1.531(2)	C–C–C	113.8(4)
C–H	1.117(5)	C–C–H (average)	111.0(5)
		C–C–C–C (<i>gauche</i>)	64.9(60) ^b

The molecule exists as a mixture of *anti* (53.5(90)%) and *gauche* conformers.

$\Delta G^0(\textit{gauche} - \textit{anti}) = 497(220) \text{ cal mol}^{-1}$.

The nozzle was at room temperature.

^a) Three times the estimated standard errors including a systematic error.

^b) Uncertainty represents 2.5 times the least-squares estimate.

Bradford, W.F., Fitzwater, S., Bartell, L.S.: J. Mol. Struct. **38** (1977) 185.

See also: Heenan, R.K., Bartell, L.S.: J. Chem. Phys. **78** (1983) 1270.