

1735
ED

C₄H₈O

2-Butanone
Ethyl methyl ketone

C_s (*anti*)
C₁ (*gauche*)
H₃C–CH₂–C(O)–CH₃

r_{α}	Å ^{a)}	θ_{α}	deg ^{a)}
C(2)=O	1.2186(12)	O=C(2)–C(3)	121.3(7)
C(1)–C(2)	1.518 ^{b)}	O=C(2)–C(1)	122.6(10)
C(2)–C(3)	1.518 ^{b)}	C(2)–C(3)–C(4)	113.5(7)
C(3)–C(4)	1.531 ^{b)}	C–C–H	113.1(9)
C–H	1.102 ^{b)}	H–C(3)–H	108.8 ^{b)}
		C(1)–C(2)–C(3)–C(4) (<i>anti</i>)	180 ^{b)}
		C(1)–C(2)–C(3)–C(4) (<i>gauche</i>)	70 ^{b)}

The molecule exists as a mixture of *anti* (95(3)%) and *gauche* (5(3)%) conformers.

The measurements were made at room temperature.

^{a)} Estimated standard errors.

^{b)} Assumed.

Abe, M., Kuchitsu, K., Shimanouchi, T.: J. Mol. Struct. **4** (1969) 245.

