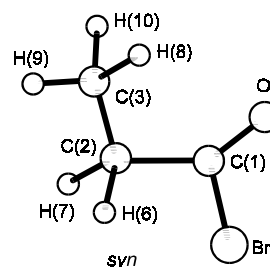


r_g	\AA^a	θ_α	deg^a
C–H	1.109(9)	C–C=O	126.6(6)
C=O	1.182(5)	C–C–Br	112.5(4)
C–C (average)	1.523(4)	C–C–C	118.8(9)
C–Br	1.979(5)	C(1)–C(2)–H(6)	110 ^{b)}
		H(6)–C(2)–H(7)	109 ^{b)}
		C(2)–C(3)–H	109 ^{b)}
		ϕ_1 ^{c)}	101(9)
		ϕ_2 ^{d)}	60 ^{b)}



The molecule exists as a mixture of *syn* and *gauche* conformers. The mole fraction of the *syn* form, with uncertainties estimated at 2σ , was found to be 0.71(10), 0.58(13), and 0.51(16) at 293, 373, and 473 K, respectively, and corresponds to $\Delta E^\circ = E^\circ(\textit{gauche}) - E^\circ(\textit{syn}) = 5.5 \text{ kJ mol}^{-1}$ ($\sigma = 2.5$) and $\Delta S^\circ = S^\circ(\textit{gauche}) - S^\circ(\textit{syn}) = 6 \text{ J mol}^{-1} \text{ K}^{-1}$ ($\sigma = 7$).

^{a)} Twice the estimated standard errors including the scale error.

^{b)} Assumed.

^{c)} O=C–C–C torsion angle in the *gauche* conformer, $\phi_1 = 0^\circ$ for *syn* conformer.

^{d)} C(1)–C(2)–C(3)–H(8) torsion angle, $\phi_2 = 0^\circ$ when C(3)–H(8) is eclipsed with respect to the C(2)–C(1).

Skjørholm, S.J., Hagen, K.: J. Phys. Chem. **91** (1987) 3977.