

1314 C₃H₇IED, MW, *ab initio*

calculations (HF/LANL1DZ)

r_g	Å ^{a)}
C(1)–C(2)	1.521(5)
C(2)–C(3)	1.537(5)
C(1)–I	2.164(8)
C–H (mean)	1.110(4)

1-Iodopropane

Propyl iodide

θ_α	deg ^{a)}
C–C–C (<i>anti</i>)	110.2(9)
C–C–C (<i>gauche</i>)	113.9(9)
C–C–I (<i>anti</i>)	111.8(4)
C–C–I (<i>gauche</i>)	113.0(4)
C(2)–C(1)–H	112.5 ^{b)}
C(2)–C(3)–H	111.0 ^{b)}
H–C(2)–H	109.5 ^{b)}
C–C–C–I (<i>anti</i>)	180
C–C–C–I (<i>gauche</i>)	66.1(5)

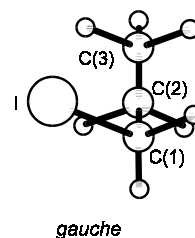
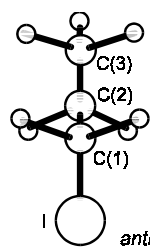
C_s (*anti*)
 C₁ (*gauche*)
 IH₂C–CH₂–CH₃

Two conformers, *gauche* (72(13)%) and *anti*, have been observed. Local C_{3v} symmetry was assumed for the methyl group.

The nozzle temperature was 25 °C.

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

^{b)} *Ab initio* value.



Hagen, K., Stølevik, R., Sæbø, P.C. : J. Mol. Struct. **346** (1995) 75.