

1778  
ED, MW

**C<sub>4</sub>H<sub>9</sub>Cl**

**Isobutyl chloride**  
1-Chloro-2-methylpropane

C<sub>1</sub> (*gauche*)  
C<sub>1</sub> (*anti*)  
ClH<sub>2</sub>C–CH(CH<sub>3</sub>)<sub>2</sub>

| $r_g$         | Å <sup>a)</sup> | $\theta_\alpha$                        | deg <sup>a)</sup>   |
|---------------|-----------------|--|---------------------|
| C–C (average) | 1.532(2)        | C–C–Cl ( <i>gauche</i> )               | 114.0(9)            |
| C–Cl          | 1.791(3)        | C–C–Cl ( <i>anti</i> )                 | 111.1(7)            |
| C–H (average) | 1.111(4)        | C(1)–C(2)–C(3) ( <i>gauche</i> )       | 111.8 <sup>b)</sup> |
|               |                 | C(1)–C(2)–C(3) ( <i>anti</i> )         | 109.3(7)            |
|               |                 | C(1)–C(2)–C(4) ( <i>gauche</i> )       | 111.8 <sup>b)</sup> |
|               |                 | C(1)–C(2)–C(4) ( <i>anti</i> )         | 114.3 <sup>b)</sup> |
|               |                 | C(3)–C(2)–C(4) <sup>c)</sup>           | 109.0(7)            |
|               |                 | Cl–C–H (average)                       | 105.9(25)           |
|               |                 | C–C(3,4)–H (average)                   | 113.1(12)           |
|               |                 | C–C(1)–H                               | 112.5 <sup>d)</sup> |
|               |                 | C(3,4)–C(2)–H                          | 109.5 <sup>d)</sup> |
|               |                 | $\tau$ ( <i>anti</i> ) <sup>e)</sup>   | –172(3)             |
|               |                 | $\tau$ ( <i>gauche</i> ) <sup>e)</sup> | 68(3)               |

Data were found to be consistent with a conformational mixture containing 62(15)% of the *anti* conformer which has a statistical weight of two, and 38(15)% of the *gauche* conformer.

This equilibrium mixture corresponds to a free energy difference

$$\Delta G = G(\text{anti}) - G(\text{gauche}) = 0.5(16) \text{ kJ mol}^{-1}.$$

The nozzle temperature was 28 °C.

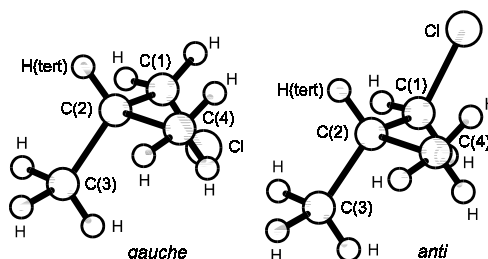
<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Value relative to C(1)–C(2)–C(3) (*anti*) estimated by systematic variations.

<sup>c)</sup> Equal value for both conformers.

<sup>d)</sup> Assumed.

<sup>e)</sup> C(3)–C(2)–C(1)–Cl dihedral angle,  $\tau = 0^\circ$  for the *syn* position.



Schei, S.H., Hilderbrandt, R.L.: J. Mol. Struct. **128** (1985) 181.

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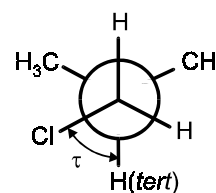
| $r_0$               | Å <sup>a)</sup>     | $\theta_0$            | deg <sup>a)</sup>   |
|---------------------|---------------------|-----------------------|---------------------|
| C–C                 | 1.532 <sup>b)</sup> | C–C–Cl                | 112(2)              |
| C–Cl                | 1.77(6)             | C–C–C                 | 110.8 <sup>b)</sup> |
| C–H ( <i>tert</i> ) | 1.109 <sup>b)</sup> | C–C–H ( <i>tert</i> ) | 108.1 <sup>b)</sup> |
| C–H ( <i>prim</i> ) | 1.092 <sup>b)</sup> | C–C–H ( <i>prim</i> ) | 111 <sup>b)</sup>   |
|                     |                     | $\tau$ <sup>c)</sup>  | 50(5)               |

<sup>a)</sup> Uncertainties are about twice those of the original data.

<sup>b)</sup> Assumed.

<sup>c)</sup> Dihedral angle H–C–C–Cl.

C<sub>1</sub> (*gauche*)



Brooks, W.V.F., Gosselin, J.A., Mohammadi, M.A., Thibault, J.D.: J. Mol. Struct. **72** (1981) 17.