

1303  
MW

**C<sub>3</sub>H<sub>7</sub>ClO**

**Chloromethyl ethyl ether**

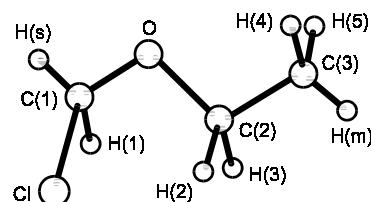
**C<sub>1</sub>**  
**ClH<sub>2</sub>C–O–CH<sub>2</sub>–CH<sub>3</sub>**

| $r_s$     | Å         | $\theta_s$     | deg       |
|-----------|-----------|----------------|-----------|
| C–Cl      | 1.829(11) | Cl–C–O         | 113.1(9)  |
| O–C(1)    | 1.347(16) | C–O–C          | 114.4(14) |
| O–C(2)    | 1.431(14) | O–C–C          | 108.1(10) |
| C(2)–C(3) | 1.514(13) | Cl–C–H(1)      | 102.8(15) |
| C(1)–H(1) | 1.100(31) | Cl–C–H(s)      | 104.4(10) |
| C(1)–H(s) | 1.092(18) | O–C(1)–H(1)    | 114.6(22) |
| C(2)–H(2) | 1.225(15) | O–C(1)–H(s)    | 110.1(14) |
| C(2)–H(3) | 1.138(45) | H(1)–C–H(s)    | 111.2(26) |
| C(3)–H(4) | 1.077(17) | O–C(2)–H(2)    | 104.0(11) |
| C(3)–H(5) | 1.092(28) | O–C(2)–H(3)    | 104.8(32) |
| C(3)–H(m) | 1.085(20) | C(3)–C(2)–H(2) | 118.8(15) |
|           |           | C(3)–C(2)–H(3) | 109.2(34) |
|           |           | H(2)–C–H(3)    | 110.9(76) |
|           |           | C(2)–C(3)–H(4) | 110.1(17) |
|           |           | C(2)–C(3)–H(5) | 110.1(17) |
|           |           | C(2)–C(3)–H(m) | 110.5(13) |
|           |           | H(4)–C–H(m)    | 107.6(25) |
|           |           | H(5)–C–H(m)    | 107.8(28) |
|           |           | H(4)–C–H(5)    | 110.7(39) |
|           |           | $\tau_1^a$     | 71.8(26)  |
|           |           | $\tau_2^b$     | 175.7(33) |

| Atom | $a_s$ [Å] | $b_s$ [Å] | $c_s$ [Å] |
|------|-----------|-----------|-----------|
| Cl   | –1.7842   | 0.4133    | –0.0443   |
| C(1) | –0.5928   | –0.9500   | –0.0677   |
| H(1) | –0.6225   | –1.0956   | 1.2817    |
| H(s) | –1.0339   | –1.8002   | –0.3327   |
| O    | 0.6310    | –0.6843   | –0.3052   |
| C(2) | 1.3701    | 0.2929    | 0.4336    |
| H(2) | 0.6439    | 1.2789    | 0.4300    |
| H(3) | 1.4597    | –0.1417   | 1.4816    |
| C(3) | 2.7498    | 0.4018    | –0.1798   |
| H(4) | 3.2662    | –0.5402   | –0.0999   |
| H(5) | 2.6732    | 0.7117    | –1.2241   |
| H(m) | 3.3404    | 1.1456    | 0.3447    |

<sup>a</sup>) Dihedral angle Cl–C–O–C.

<sup>b</sup>) Dihedral angle C–C–O–C.



Hayashi, M., Kato, H.: Bull. Chem. Soc. Jpn. **53** (1980) 2701.