

| r_0 | Å | θ_0 | deg ^{a)} |
|------------|----------|------------------------|-------------------|
| C(1)–C(2) | 1.470(3) | O(4)–C(1)–C(2) | 59.1(2) |
| C(2)–C(3) | 1.505(2) | O(4)–C(2)–C(1) | 59.4(1) |
| C(1)–O(4) | 1.441(2) | C(1)–O(4)–C(2) | 61.5(2) |
| C(2)–O(4) | 1.435(3) | C(1)–C(2)–C(3) | 121.7(2) |
| C(1)–H(5) | 1.088(2) | O(4)–C(2)–C(3) | 116.1(2) |
| C(1)–H(6) | 1.082(2) | H(5)–C(1)–O(4) | 114.4(2) |
| C(2)–H(7) | 1.087(1) | H(6)–C(1)–O(4) | 114.8(1) |
| C(3)–H(8) | 1.095(3) | H(7)–C(2)–O(4) | 114.8(3) |
| C(3)–H(9) | 1.092(2) | H(5)–C(1)–C(2) | 118.3(1) |
| C(3)–H(10) | 1.090(3) | H(6)–C(1)–C(2) | 120.1(2) |
| | | H(7)–C(2)–C(1) | 118.5(3) |
| | | H(5)–C(1)–H(6) | 116.7(2) |
| | | C(3)–C(2)–H(7) | 114.5(2) |
| | | C(2)–C(3)–H(8) | 110.0(3) |
| | | C(2)–C(3)–H(9) | 109.8(1) |
| | | C(2)–C(3)–H(10) | 110.5(4) |
| | | H(8)–C(3)–H(9) | 109.2(5) |
| | | H(9)–C(3)–H(10) | 109.2(8) |
| | | H(10)–C(3)–H(8) | 108.1(3) |
| | | τ_1 ^{a)} | –44.0(5) |
| | | τ_2 ^{b)} | 24.7(8) |
| | | τ_3 ^{c)} | –95.5(5) |
| | | τ_4 ^{d)} | 145.2(12) |

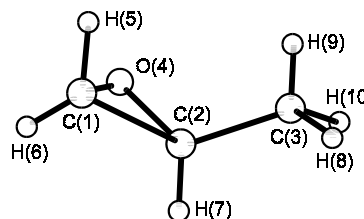
| Atom | a_0 [Å] | b_0 [Å] | c_0 [Å] |
|-------|-----------|-----------|-----------|
| C(1) | 0.9612 | –0.6943 | –0.1151 |
| C(2) | –0.2101 | –0.0447 | 0.4917 |
| C(3) | –1.5550 | –0.0483 | –0.1846 |
| O(4) | 0.8122 | 0.7383 | –0.1411 |
| H(5) | 0.8388 | –1.1772 | –1.0825 |
| H(6) | 1.7663 | –1.0560 | 0.5116 |
| H(7) | –0.2492 | 0.0468 | 1.5741 |
| H(8) | –2.1654 | –0.8717 | 0.2001 |
| H(9) | –1.4265 | –0.1693 | –1.2625 |
| H(10) | –2.0827 | 0.8846 | 0.0115 |

^{a)} Dihedral angle O(4)–C(2)–C(3)–H(9).

^{b)} Dihedral angle C(1)–C(2)–C(3)–H(9).

^{c)} Dihedral angle C(1)–C(2)–C(3)–H(8).

^{d)} Dihedral angle C(1)–C(2)–C(3)–H(10).



Imachi, M., Kuczkowski, R.L.: J. Mol. Struct. **96** (1982) 55.

See also: Andresen, U., Rudolph, H.D.: Z. Naturforsch. **26a** (1971) 320.