

1671
MW

C₄H₆O₃

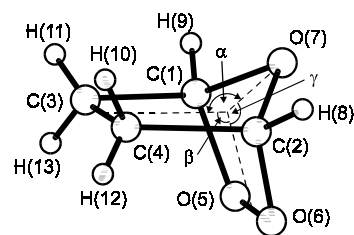
2,3,7-Trioxabicyclo[2.2.1]heptane

C_s



r_s	Å	θ_s	deg
C(1)–O(5)	1.418(5)	C(1)–C(3)–C(4)	99.5(3)
C(1)–O(7)	1.417(5)	C(1)–O(5)–O(6)	101.8(3)
C(1)–C(3)	1.546(5)	C(1)–O(7)–C(2)	94.0(3)
C(3)–C(4)	1.561(15)	C(3)–C(1)–O(7)	104.4(3)
O(5)–O(6)	1.492(5)	C(3)–C(1)–O(5)	108.8(3)
C(1)–H(9)	1.095(5)	O(7)–C(1)–O(5)	103.4(5)
C(3)–H(11)	1.104(15)	H(9)–C(1)–C(3)	99.5(15)
C(3)–H(13)	1.080(15)	H(9)–C(1)–O(5)	126.2(10)
		H(9)–C(1)–O(7)	112.6(10)
		H(11)–C(3)–C(1)	109.6(10)
		H(11)–C(3)–C(4)	111.7(10)
		H(11)–C(3)–H(13)	110.8(15)
		H(13)–C(3)–C(1)	111.3(10)
		H(13)–C(3)–C(4)	113.4(10)
		α^a	123.3(10)
		β^b	111.7(3)
		γ^c	124.9(10)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(1,2)	–0.0294	±1.0344	0.3279
C(3,4)	1.2782	±0.7854	–0.4644
O(5,6)	–1.1327	±0.7445	–0.5091
O(7)	–0.0568	0.0	1.2920
H(8,9)	0.1854	±2.0108	0.7763
H(10,11)	2.1353	±1.1895	0.1187
H(12,13)	1.2365	±1.2064	–1.4423



^a) Angle between the C(1)O(7)C(2) and C(1)C(2)C(3)C(4) planes.

^b) Angle between the C(1)C(2)C(3)C(4) and C(1)C(2)O(6)O(5) planes.

^c) Angle between the C(1)O(7)C(2) and C(1)C(2)O(6)O(5) planes.

Borseth, D.G., Lorencak, P., Badawi, H.M., Hillig, K.W., Kuczkowski, R.L., Mendenhall, G.D.:
J. Mol. Struct. **190** (1988) 125.