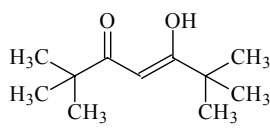


900
ED $C_{11}H_{20}O_2$ **(4Z)-5-Hydroxy-2,2,6,6-tetramethyl-4-hepten-3-one**
2,2,6,6-Tetramethylheptan-3,5-dione, (Z)-enol form C_{2v}

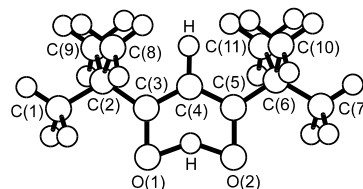
r_g	\AA^a	θ_α	deg^a	
C(4)–C(3,5)	1.449(6)	C–C(4)–H	119.7(4)	
C(1)–C(2)	1.558(4)	C(4)–C–O	117.6(4)	
C(2)–C(3)	1.526(4)	C–O–H	75(4)	
C–O	1.277(6)	C(1)–C(2)–C(3)	108.0(2)	
C–H(methyl)	1.129(5)	C(2)–C(3)–C(4)	113.6(6)	
O–H	1.285(25)	C(3)–C(4)–C(5)	120.6(4)	
O...O	2.405(18)	C–C–H(methyl)	110.1(6)	
C(4)–H	1.10 ^{b)}	O–H–O	146(6)	

Only monomeric molecules were detected in the vapor by mass spectrometric method. Two molecular models of C_{2v} and C_s symmetry were considered in the ED analysis. The more symmetric model with the enol hydrogen lying symmetrically relative to the oxygen atoms was preferred to the classical model of the enol tautomer. It was assumed that the OCCCCO fragment is planar and the *t*-butyl and methyl groups have local C_{3v} symmetry. The *t*-butyl groups of the C_{2v} model were found to be in the staggered position with respect to the C(4)–C bonds.

The nozzle was at 24(3) °C.

^{a)} 2.5 times the estimated standard errors including a systematic error.

^{b)} Assumed.



Giricheva, N.I., Girichev, G.V., Lapshina, S.B., Kuzmina, N.I.: Zh. Strukt. Khim. **41** No.1 (2000) 58; J. Struct. Chem. (Engl. Transl.) **41** (2000) 48.