

1351
MW

C₃H₈O₂

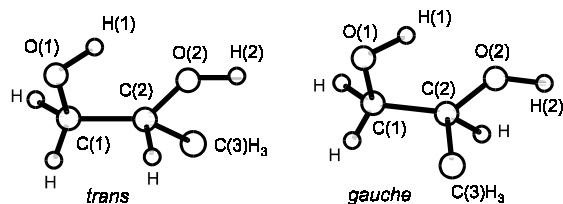
1,2-Propanediol

C₁ (*trans*)
C₁ (*gauche*)
HO-CH₂-CH(OH)-CH₃

r_0	\AA^a	
	<i>trans</i>	<i>gauche</i>
C-C	1.54 ^{b)}	1.54 ^{b)}
C-O	1.42 ^{b)}	1.42 ^{b)}
C-H	1.095 ^{b)}	1.095 ^{b)}
O-H	1.00 ^{b)}	1.00 ^{b)}

θ_0	deg^a	
	<i>trans</i>	<i>gauche</i>
C-C-C	112.2(10)	108.9(20)
C-O-H	108 ^{b)}	108 ^{b)}
C-C-O	108.1(10)	110.0(10)
C-C-H	109.5 ^{b)}	109.5 ^{b)}
$\tau_1^c)$	45.8(40)	47.9(40)
$\tau_2^d)$	58.4(20)	53.0(20)
$\tau_3^e)$	166.4(40)	183.7(40)

Two conformations *trans* and *gauche* are detected, i.e. C(1)-O(1) and C(2)-C(3) are *trans* and *gauche* with respect to C(1)-C(2). The *trans* form is more stable than the *gauche* form by 0.58 kcal mol⁻¹.



^{a)} Uncertainties are about twice those of the original data.

^{b)} Assumed.

^{c)} Dihedral angle H(1)-O(1)-C(1)-C(2).

^{d)} Dihedral angle O(1)-C(1)-C(2)-O(2).

^{e)} Dihedral angle H(2)-O(2)-C(2)-C(1).

Caminati, W.: J. Mol. Spectrosc. **86** (1981) 193.