

1352
ED

C₃H₈O₂

1,3-Propanediol

C₁ (*gauche*⁺–*gauche*[–])
HO–CH₂–CH₂–CH₂–OH

<i>r</i> _a	Å ^{a)}	<i>θ</i> _a	deg ^{a)}
C–C	1.514(8)	C–C–C	112.0(15)
C–O	1.410(6)	C–C–O(1)	108.0(15)
C–H	1.140(2)	C–C–O(2)	112.0(15)
O(1)–H	1.04(7)	C–O(1)–H	109(3)
O(2)–H	0.98(6)	C–O(2)–H	97(3)
		C–C–H	109 ^{b)}
		τ ₁ ^{c)}	68(3)
		τ ₂ ^{d)}	61(5)
		τ ₃ ^{e)}	46(5)
		τ ₄ ^{f)}	108 ^{b)}

The conformation is *gauche*⁺–*gauche*[–] with the O...O distance of 2.70 Å forming an internal hydrogen bridge.

The nozzle temperature was 167 °C.

^{a)} Three times the estimated standard errors.

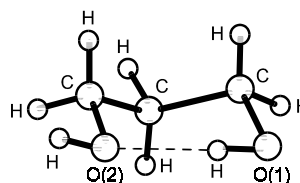
^{b)} Assumed.

^{c)} Dihedral angle O(1)–C–C–C.

^{d)} Dihedral angle O(2)–C–C–C.

^{e)} Dihedral angle C–C–O(1)–H.

^{f)} Dihedral angle C–C–O(2)–H.



Kinneging, A.J., Mom, V., Mijlhoff, F.C., Renes, G.H.: J. Mol. Struct. **82** (1982) 271.