

1818
MW

C₄H₁₀O

Isopropyl methyl ether

C₁
H₃C–O–CH(CH₃)₂

r_0	Å ^{a)}	θ_0	deg ^{a)}
O–C(4)	1.416(5)	C–O–C	112.5(5)
O–C(3)	1.422(5)	O–C(3)–C(1)	113.7(5)
C(3)–C(2)	1.528(5)	O–C(3)–C(2)	107.7(5)
C(3)–C(1)	1.519(5)	C–C–C	112.7 ^{b)}
C(1,2)–H	1.090 ^{b)}	τ_1 ^{c)}	71.9 ^{b)}
C(3)–H	1.095 ^{b)}	τ_2 ^{d)}	162.6 ^{b)}
C(4)–H	1.095 ^{b)}	τ_3 ^{e)}	47.0(10)

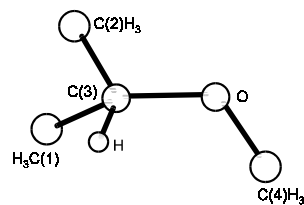
^{a)} Uncertainties were not estimated in the original paper.

^{b)} Assumed.

^{c)} Dihedral angle C–O–C–C(1).

^{d)} Dihedral angle C–O–C–C(2).

^{e)} Dihedral angle C(4)–O–C(3)–H.



Nakagawa, J., Imachi, M., Hayashi, M.: J. Mol. Struct. **112** (1984) 201.