

1345
MW

C₃H₈O

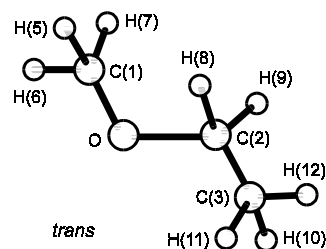
Ethyl methyl ether

C_s (*trans*)
C₁ (*gauche*)
H₃C–O–CH₂–CH₃

trans

<i>r_s</i>	Å	<i>θ_s</i>	deg
C(3)–C(2)	1.521(7)	C–O–C	111.7(5)
C(2)–O	1.407(4)	C–C–O	108.2(4)
C(1)–O	1.415(5)	C(3)–C(2)–H	110.3(9)
C(2)–H	1.100(3)	O–C(2)–H	110.3(5)
C(3)–H(s)	1.089(8)	H–C(2)–H	107.4(3)
C(3)–H(a)	1.092(7)	O–C(1)–H(s)	107.5(6)
C(1)–H(s)	1.086(10)	O–C(1)–H(a)	111.1(5)
C(1)–H(a)	1.099(7)	H(s)–C(1)–H(a)	109.3(8)
		H(a)–C(1)–H(a)	108.6(6)
		<i>γ</i> ₁ ^{a)}	109.9(5)
		<i>δ</i> ₁ ^{b)}	2.4(5)
		C(2)–C(3)–H(s)	110.5(6)
		C(2)–C(3)–H(a)	110.1(6)
		H(s)–C(3)–H(a)	108.7(7)
		H(a)–C(3)–H(a)	108.6(6)
		<i>γ</i> ₂ ^{c)}	110.3(6)
		<i>δ</i> ₂ ^{d)}	–0.3(6)

Atom	<i>a_s</i> [Å]	<i>b_s</i> [Å]	<i>c_s</i> [Å]
C(3)	–1.8603	–0.1584	0.0
C(2)	–0.5027	0.5263	0.0
O	0.4908	–0.4698	0.0
C(1)	1.7909	0.0880	0.0
H(12)	–2.6601	0.5804	0.0
H(10,11)	–1.9643	–0.7867	±0.8868
H(8,9)	–0.3992	1.1694	±0.8868
H(6)	2.4992	–0.7351	0.0
H(5,7)	1.9545	0.7058	±0.8928



^{a)} The corrected O–C(1)–H value defined by $\gamma_1 = (1/3) [(O-C(1)-H(s)) + 2(O-C(1)-H(a))]$.

^{b)} The tilt angle of the C(1)H₃ group defined by $\delta_1 = (2/3) [(O-C(1)-H(a)) - (O-C(1)-H(s))]$.

^{c)} The corrected C–C(3)–H value defined by $\gamma_2 = (1/3) [(C-C(3)-H(s)) + 2(C-C(3)-H(a))]$.

^{d)} The tilt angle of the C(3)H₃ group defined by $\delta_2 = (2/3) [(C-C(3)-H(a)) - (C-C(3)-H(s))]$.

Hayashi, M., Adachi, M.: J. Mol. Struct. **78** (1982) 53.

ED, MW

<i>r_g</i>	Å ^{a)}	<i>θ_α</i>	deg ^{a)}
C–C	1.520(4)	C–O–C	111.9(5)
C–O (average)	1.418(2)	C–C–O	109.4(3)
C(2)–O	1.422(7)	H–C–H	109.0(4)
C(1)–O	1.413(9)	<i>τ</i> ^{b)}	84(6)
C–H (average)	1.118(4)		

Abundance of the *trans* conformer was 80(8)%. $\Delta G(\textit{gauche} - \textit{trans}) = 1.23(27)$ kcal mol^{–1}.

The nozzle was at room temperature.

^{a)} Estimated limits of error.

^{b)} Dihedral angle C(1)–O–C(2)–C(3) for the *gauche* conformer measured from the *syn* position.

Oyanagi, K., Kuchitsu, K.: Bull. Chem. Soc. Jpn. **51** (1978) 2237.

