

1329
MW

C₃H₇NO₂

Propyl nitrite

C_s (*cis-trans-trans*)
C₁ (*cis-gauche-gauche*)
H₃C-CH₂-CH₂-O-N=O

r_0	Å	θ_0	deg
C-H	1.094 ^{a)}	C-C-C	112.7 ^{a)}
C(1)-C(2)	1.509 ^{a)}	C-C-O	109.5 ^{a)}
C(2)-C(3)	1.523 ^{a)}	H-C-C	109.5 ^{a)}
C-O	1.436 ^{a)}	H-C-H	109.5 ^{a)}
O-N	1.386 ^{a)}	C-O-N	114.2(28)
N=O	1.180 ^{a)}	O-N=O	122.8(50)
		C-O-N=O (<i>cis</i>)	0 ^{a)}
		C-C-O-N (<i>gauche</i>)	79.9(34)
		C-C-C-O (<i>gauche</i>)	74.6(80)

There are two conformers; one is *cis-trans-trans* and the other *cis-gauche-gauche* about the O-N, C(1)-O, C(2)-C(1) bonds, respectively.

^{a)} Assumed.

Endo, K., Furuhashi, A.: Nippon Kagaku Kaishi (1987) 2227.

See also: Endo, K., Tanuma, R., Sekine, A., Kamura, Y.: Nippon Kagaku Kaishi (1986) 1051.

