

1704
MW

C₄H₇NO

Propyl isocyanate

C₁ (conformer I)
C_s (conformer II)
H₃C–CH₂–CH₂–N=C=O

<i>r</i> ₀	Å	<i>θ</i> ₀	deg
C=O	1.171 ^{a)}	N=C=O	180.0 ^{a)}
C=N	1.207 ^{a)}	N–C–H	109.5 ^{a)}
C–N	1.426 ^{a)}	C(2)–C(3)–H	109.5 ^{a)}
C–H	1.094 ^{a)}	C(3)–C(4)–H	110.14 ^{a)}
C(4)–C(3)	1.544 ^{a)}		
C(3)–C(2)	1.536 ^{a)}		
		conformer I	conformer II
		N–C(2)–C(3)	111.5 ^{a)} 110.5 ^{a)}
		C(2)–C(3)–C(4)	111.5 ^{a)} 110.5 ^{a)}
		C(1)–N–C(2)	148.0(10) 143.5(10)
		<i>τ</i> ₁ ^{b)}	60.0(20) 180.0(20)
		<i>τ</i> ₂ ^{c)}	0.0(20) 0.0(20)

^{a)} Assumed.

^{b)} Dihedral angle N–C(2)–C(3)–C(4).

^{c)} Dihedral angle C(1)=N–C(2)–C(3).

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