

1255  
MW

**C<sub>3</sub>H<sub>6</sub>NP**

**3-Phosphinopropionitrile**

C<sub>1</sub> (*gauche* II)

C<sub>1</sub> (*anti* IV)

C<sub>s</sub> (*anti* V)

H<sub>2</sub>P-CH<sub>2</sub>-CH<sub>2</sub>-C≡N

$r_0$	Å	$\theta_0$	deg			
C-P	1.880 <sup>a)</sup>	C-C≡N	180.00 <sup>a)</sup>			
C≡N	1.157 <sup>a)</sup>	C-C-C	110.50 <sup>a)</sup>			
C(1)-C(2)	1.530 <sup>a)</sup>	C-P-H	95.50 <sup>a)</sup>			
C(2)-C(3)	1.474 <sup>a)</sup>	H-P-H	93.40 <sup>a)</sup>			
P-H	1.414 <sup>a)</sup>	C-C-H	109.48 <sup>a)</sup>			
C-H	1.093 <sup>a)</sup>	H-C-H	109.48 <sup>a)</sup>			
		<i>anti</i> IV		<i>anti</i> V	<i>gauche</i> II	
		C-C-P	109.0(15)	114.0(15)	117.0(15)	
		$\tau$ <sup>b)</sup>	180	180	66(3)	

*Gauche* II form is more stable than *anti* V form by 0.3(20) kJ mol<sup>-1</sup>, and *anti* V form is more stable than *anti* IV form by 3(2) kJ mol<sup>-1</sup>.

<sup>a)</sup> Assumed.

<sup>b)</sup> Dihedral angle  
C-C-C-P from *syn*.

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