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MW

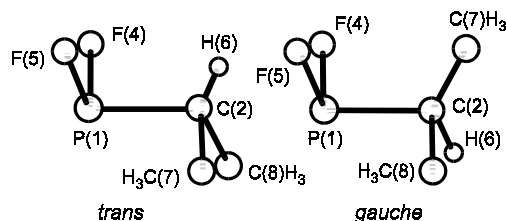
**C<sub>3</sub>H<sub>7</sub>F<sub>2</sub>P**

**Difluoroisopropylphosphine**

C<sub>1</sub> (*gauche*)  
C<sub>s</sub> (*trans*)  
F<sub>2</sub>P–CH(CH<sub>3</sub>)<sub>2</sub>

<i>r</i> <sub>0</sub>	Å	
	<i>gauche</i>	<i>trans</i>
P–C	1.8279(40)	1.842(30)
P–F(4,5)	1.5984(20)	1.585(18)
C–C(7,8)	1.535 <sup>a</sup>	1.535 <sup>a</sup>
C–H(6)	1.093 <sup>a</sup>	1.093 <sup>a</sup>
C(7,8)–H	1.093 <sup>a</sup>	1.093 <sup>a</sup>

<i>θ</i> <sub>0</sub>	deg	
	<i>gauche</i>	<i>trans</i>
C–P–F(4)	98.52(12)	97.94(80)
C–P–F(5)	100.72(16)	97.94(80)
P–C–H(6)	103.22(10)	106.1(12)
P–C–C(7)	113.55(11)	108.73(18)
P–C–C(8)	107.62(5)	108.73(18)
C–C(7,8)–H	110.48(2)	110.93(26)
F–P–F <sup>b</sup>	95.78(19)	98.8(13)
C–C–C <sup>b</sup>	112.04(6)	111.00(45)
H(6)–C–C(7) <sup>b</sup>	108.50(15)	111.05(51)
H(6)–C–C(8) <sup>b</sup>	111.62(13)	111.05(51)
(1/2)(P–F–C–F)	48.79(8)	50.06(53)
H(6)–C–P–d(3) <sup>c</sup>	117.85(14)	0 <sup>a</sup>
C(7)–C–P–d(3) <sup>c</sup>	0.60(4)	119.52(28)
C(8)–C–P–d(3) <sup>c</sup>	–124.0 <sup>a</sup>	119.52(28)



The *gauche* conformer is more stable than *trans* by 33(7) cm<sup>–1</sup> in the liquid phase.

<sup>a</sup>) Assumed.

<sup>b</sup>) Dependent parameter.

<sup>c</sup>) d(3) represents a dummy atom halfway between the F atoms.

Durig, J.R., Cheng, M.S., Li, Y.S., Groner, P., Stanley, A.E.: J. Phys. Chem. **93** (1989) 3492.  
See also: Stanley, A.E., Durig, J.R., Li, Y.S.: 11th Austin Symp. Mol. Struct. 1986, MM9.