

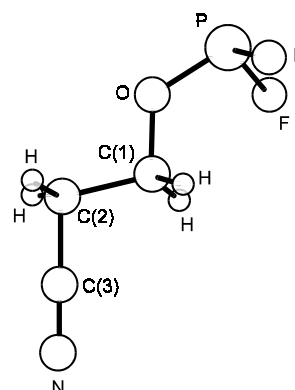
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C₃H₄F₂NOP

3-(Difluorophosphinoxy)propionitrile

essentially C_s
F₂P–O–CH₂–CH₂–C≡N

r_a	Å ^{a)}	θ_a	deg ^{a)}
P–F	1.601(3)	C–C–O	106.2(11)
P–O	1.551(8)	C–C–C	106.7(7)
O–C	1.406(8)	F–P–F	93.6(9)
N≡C	1.183(4)	O–P–F	102.0(4)
C–H	1.085(12)	C–O–P	121.9(8)
C(1)–C(2)	1.540 ^{b)}	C–C–H	109.0 ^{b)}
C(2)–C(3)	1.504(10)	H–C–H	109.0 ^{b)}
		$\tau^c)$	19.2(14)



The PF₂O and C≡N groups are *anti* with respect to each other.
The nozzle temperature was 313 K.

^{a)} Estimated standard errors including a systematic error.

^{b)} Assumed.

^{c)} Torsional angle of the PF₂ group about the P–O bond; $\tau = 0^\circ$ when the F–P–F angle bisector is *syn* to the O–C bond. The deviation from 0° is probably caused by the effects of the torsional vibration.

Blake, A.J., Davis, M.J., Rankin, D.W.H.: J. Mol. Struct. **221** (1990) 25.