

1358
MW

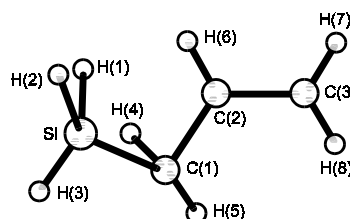
C₃H₈Si

Allylsilane

C₁ (skew)
H₂C=CH-CH₂-SiH₃

r_s	Å	θ_s	deg
C(2)=C(3)	1.328(7)	C(1)-C(2)=C(3)	126.7(8)
C(1)-C(2)	1.492(8)	C(2)-C(1)-Si	111.6(5)
C(1)-Si	1.875(4)	H-C(3)-H	117.1(3)
C(3)-H(7)	1.074(2)	H(7)-C(3)=C(2)	123.1(8)
C(3)-H(8)	1.094(3)	H(8)-C(3)=C(2)	119.7(9)
C(2)-H(6)	1.102(9)	C(2)-C(1)-H(4)	113.0(8)
C(1)-H(4)	1.100(2)	C(2)-C(1)-H(5)	106.6(8)
C(1)-H(5)	1.122(4)	H(4)-C(1)-Si	110.3(5)
Si-H(1)	1.496(3)	H(5)-C(1)-Si	110.3(4)
Si-H(2)	1.480(4)	H-C(3)-H	104.6(4)
Si-H(3)	1.478(2)	C(1)-Si-H(1)	108.5(3)
		C(1)-Si-H(2)	108.8(3)
		C(1)-Si-H(3)	110.5(2)
		H(1,2)-Si-H(3)	110.5(2)
		H(1)-Si-H(2)	107.9(2)
		τ^a	106.8(11)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
C(3)	-2.2264	-0.4084	-0.2215
H(7)	-3.0474	-0.8956	0.2700
H(8)	-2.2612	-0.3520	-1.3135
C(2)	-1.2125	0.1446	0.4336
H(6)	-1.2433	0.1446	1.5349
C(1)	-0.0226	0.8156	-0.1666
H(4)	0.1575	1.8202	0.2435
H(5)	-0.2647	0.9900	-1.2481
Si	1.5187	-0.2399	-0.0058
H(1)	1.2943	-1.5233	-0.7402
H(2)	1.7268	-0.5642	1.4229
H(3)	2.6946	0.4699	-0.5518



^a) Dihedral angle C(3)=C(2)-C(1)-Si.

Imachi, M., Nakagawa, J., Hayashi, M.: J. Mol. Struct. **102** (1983) 403.

ED

r_a	Å ^{a)}	θ_a	deg ^{a)}
Si-C	1.875(4)	Si-C-C	113.1(4)
C-C	1.500 ^{b)}	C-C=C	125.6 ^{b)}
C=C	1.325(4)	C-Si-H	107 ^{b)}
Si-H	1.479 ^{b)}	Si-C-H	109 ^{b)}
C-H (mean)	1.090 ^{b)}	H-C-H	105 ^{b)}
		C=C-H (mean)	117(2)
		τ^c	102(1)

Temperature was estimated to be -20 °C.

^a) Estimated standard errors including a systematic error.

^b) Fixed.

^c) Torsional angle Si-C-C=C; $\tau = 0^\circ$ for the *syn* position.

Beagley, B., Foord, A., Moutran, R., Rozsondai, B.: J. Mol. Struct. **42** (1977) 117; Errata: **51** (1979) 156.