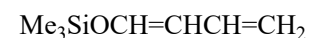




>>Entry Name: 1-Trimethylsilyloxy-1,3-butadiene

Synonym(s): (1,3-Butadienyloxy)trimethylsilane, 12Cl, 9Cl

CAS Registry Number: 6651-43-0



Molecular Formula: $\text{C}_7\text{H}_{14}\text{OSi}$

Molecular Weight: 142.272

Accurate Mass: 142.081392

Percentage Composition: C 59.10%; H 9.92%; O 11.25%; Si 19.74%

Source/Synthesis: Synth. from crotonaldehyde + Et_3N + Me_3SiCl in presence of ZnCl_2 + hydroquinone

Use/Importance: Diels-Alder diene; undergoes [2+2] cycloaddn. with dichloroketene at the remote double bond; dimerised by Ni(0) to 3,4-disubst. cyclooctadiene. Undergoes aldol condensation-type group-transfer polym.

Physical Description: Moisture-sensitive liq.

Boiling Point: Bp 131°

Density: d 0.811

Refractive Index: n_D^{20} 1.4480

Aldrich: 22722-6

Fluka: 92727

>>Variant: (E)-form

CAS Registry Number: 63383-46-0

Molecular Formula: $\text{C}_7\text{H}_{14}\text{OSi}$

Molecular Weight: 142.272

Accurate Mass: 142.081392

Percentage Composition: C 59.10%; H 9.92%; O 11.25%; Si 19.74%

Physical Description: Liq.

Boiling Point: Bp₅₆ 60°. Bp₂₅ 49.5°

Refractive Index: n_D^{20} 1.4472

>>Variant: (Z)-form

CAS Registry Number: 36045-78-0

Molecular Formula: $\text{C}_7\text{H}_{14}\text{OSi}$

Molecular Weight: 142.272

Accurate Mass: 142.081392

Percentage Composition: C 59.10%; H 9.92%; O 11.25%; Si 19.74%

Physical Description: Liq.

Boiling Point: Bp₇₄₀ 80-85°

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 1095B, (ir)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 661A, (nmr)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1642A, (ir)
Belg. Pat., 1966, 670; 769; *CA*, **65**, 5487d, (use, cycloaddn)
Cazeau, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1972, 1658-1659, (E-form, synth)
Rautenstrauch, V., *Helv. Chim. Acta*, 1972, **55**, 594-609, (Z-form, synth, ir, pmr)
Ishida, A. *et al.*, *Bull. Chem. Soc. Jpn.*, 1977, **50**, 1161-1168, (synth)
Yamamoto, K. *et al.*, *Chem. Lett.*, 1978, 649-652, (use)
Fleming, I. *et al.*, *Tet. Lett.*, 1979, 3205-3208, (use)
Fieser and Fieser's Reagents for Organic Synthesis, Wiley, 1980, **8**, 512, (use)
Brady, W.T. *et al.*, *J.O.C.*, 1981, **46**, 1322-1333, (use, cycloaddn)
Brun, P. *et al.*, *Tet. Lett.*, 1983, **24**, 385-388, (use, dimerisation)
Cazeau, P. *et al.*, *Tetrahedron*, 1987, **43**, 2089-2100, (E-form, synth, ir, pmr)
Hirabayashi, T. *et al.*, *Polym. J. (Tokyo)*, 1988, **20**, 1041-1048; 1992, **24**, 669; 1994, **26**, 705, (polym)
Rigby, J.H. *et al.*, *Tet. Lett.*, 1990, **31**, 3385-3388, (use)