



>>Entry Name: 1,4-Dichloro-2-butene, 9CI

CAS Registry Number: 764-41-0

ClCH2CH=CHCH2Cl

Molecular Formula: C₄H₆Cl₂

Molecular Weight: 124.997

Accurate Mass: 123.984654

Percentage Composition: C 38.44%; H 4.84%; Cl 56.73%

Hazard & Toxicity: Severe skin and eye irritant. LD₅₀ (rat, orl) 89 mg/kg; LD₅₀ (rbt, skn) 620 mg/kg. Exp. carcinogen and teratogen. Exp. reprod. effects

Aldrich: 15932-8

>>Variant: (E)-form

CAS Registry Number: 110-57-6

Molecular Formula: C₄H₆Cl₂

Molecular Weight: 124.997

Accurate Mass: 123.984654

Percentage Composition: C 38.44%; H 4.84%; Cl 56.73%

Physical Description: Liq.

Melting Point: Mp 1°

Boiling Point: Bp₇₅₈ 155.5°

Hazard & Toxicity: LC₅₀ (rat, ihl) 86 ppm (4h exposure)

Aldrich: 32451-5

Supelco: 44-2814

>>Variant: (Z)-form

CAS Registry Number: 1476-11-5

Molecular Formula: C₄H₆Cl₂

Molecular Weight: 124.997

Accurate Mass: 123.984654

Percentage Composition: C 38.44%; H 4.84%; Cl 56.73%

Physical Description: Liq.

Melting Point: Fp -48°

Boiling Point: Bp 152.5°. Bp₃ 22.5°

Other Data: Bp also recorded as 128°

Aldrich: 19570-7

Fluka: 35587

Supelco: 44-2526

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 146A; 146B; 146C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 100B; 100C; 100D, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 140D; 141A; 141B, (*ir*)

Registry of Mass Spectral Data, Wiley, 201-5, (*ms*)

Sadtler Standard C-13 NMR Spectra, 351, (*cmr*)

Mislow, K. *et al.*, *J.A.C.S.*, 1951, **73**, 244, (*synth, ir*)

Hecht, H.G. *et al.*, *J.A.C.S.*, 1967, **89**, 2532, (*pmr, synth*)

Sum, P.E. *et al.*, *Can. J. Chem.*, 1977, **55**, 996, (*synth*)

IARC Monog., 1977, **15**, 149; *Suppl. 7*, 62, (*rev, tox*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, BRG000; DEV000