



>>Entry Name: 3-Hexene, 9CI

Synonym(s): 3-Hexylene

CAS Registry Number: 592-47-2

Extra CAS Registry Numbers(s): 25264-93-1

H3CCH2CH=CHCH2CH3

Molecular Formula: C₆H₁₂

Molecular Weight: 84.161

Accurate Mass: 84.0939

Percentage Composition: C 85.63%; H 14.37%

>>Variant: (*E*)-form

CAS Registry Number: 13269-52-8

Molecular Formula: C₆H₁₂

Molecular Weight: 84.161

Accurate Mass: 84.0939

Percentage Composition: C 85.63%; H 14.37%

Melting Point: Fp −113°

Boiling Point: Bp₇₄₁ 67.4-67.6°

Aldrich: 44715-3

Fluka: 52990

>>Variant: (*Z*)-form

CAS Registry Number: 7642-09-3

Molecular Formula: C₆H₁₂

Molecular Weight: 84.161

Accurate Mass: 84.0939

Percentage Composition: C 85.63%; H 14.37%

Melting Point: Mp −135°

Boiling Point: Bp₇₄₁ 66.8-66.9°

Fluka: 52985

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 24C, (*nmr*)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 18A, (*ir*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 24B, (*ir*)

Lespiau, E. *et al.*, *Bull. Soc. Chim. Fr.*, 1929, **45**, 627

Campbell, K.N. *et al.*, *J.A.C.S.*, 1941, **63**, 216, (*synth*)

Mägerlein, H. *et al.*, *Chem. Ber.*, 1970, **103**, 2995, (*synth*)