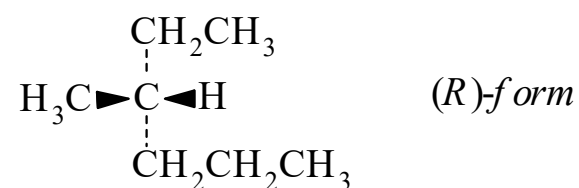




>>Entry Name: 3-Methylhexane, 9CI
Synonym(s): Ethylmethylpropylmethane



CAS Registry Number: 589-34-4

Molecular Formula: C₇H₁₆
Molecular Weight: 100.203
Accurate Mass: 100.1252
Percentage Composition: C 83.91%; H 16.09%
Hazard & Toxicity: Highly flammable, fl. p. -4°/-1°, autoignition temp. 280°

Aldrich: M4980-1
Fluka: 67370

>>Variant: (R)-form

CAS Registry Number: 78918-91-9
Molecular Formula: C₇H₁₆
Molecular Weight: 100.203
Accurate Mass: 100.1252
Percentage Composition: C 83.91%; H 16.09%
Boiling Point: Bp 92°
Optical Rotation: $[\alpha]_{\text{D}}^{21} -7.75$

>>Variant: (S)-form

CAS Registry Number: 6131-24-4
Molecular Formula: C₇H₁₆
Molecular Weight: 100.203
Accurate Mass: 100.1252
Percentage Composition: C 83.91%; H 16.09%
Boiling Point: Bp 92°
Optical Rotation: $[\alpha]_{\text{D}}^{25} +9.43$ (neat)

>>Variant: (±)-form

Molecular Formula: C₇H₁₆
Molecular Weight: 100.203
Accurate Mass: 100.1252
Percentage Composition: C 83.91%; H 16.09%
Boiling Point: Bp 91.8°
Density: d²⁰ 0.687
Refractive Index: n_D²⁰ 1.3865

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 11C, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 9B, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 11A, (*ir*)
Levene, P.A. *et al.*, *J. Biol. Chem.*, 1931, **91**, 77, (*synth*)
Heller, H.E., *J.A.C.S.*, 1952, **74**, 4858, (*synth*)
Freudenberg, K. *et al.*, *Annalen*, 1955, **594**, 76, (*abs config*)
Rossi, R. *et al.*, *Tetrahedron*, 1970, **26**, 4067, (*synth*)
Kirmse, W. *et al.*, *Chem. Ber.*, 1977, **110**, 2290, (*synth*)
Salvadori, P. *et al.*, *Tet. Lett.*, 1977, 195, (*synth*)
Sax, N.I., *Dangerous Properties of Industrial Materials, 5th edn.*, Van Nostrand Reinhold, 1979, 823
Bretherick, L., *Handbook of Reactive Chemical Hazards, 4th edn.*, Butterworths, 1990, 2691