



>>Entry Name: 2-Methylhexane

Synonym(s): Isoheptane

CAS Registry Number: 591-76-4

Related CAS Registry Numbers(s): 31394-54-4

$\text{H}_3\text{CCH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$

Molecular Formula: C_7H_{16}

Molecular Weight: 100.203

Accurate Mass: 100.1252

Percentage Composition: C 83.91%; H 16.09%

Biological Source: Found in tar oils, shales and ocean sediments. Constit. of plant spp.

Physical Description: Oil

Melting Point: Fp -119.1°

Boiling Point: Bp 90°

Hazard & Toxicity: Highly flammable, fl. p. -18° , autoignition temp. 220°

Aldrich: M4970-4

Fluka: 67360

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 11B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 9A, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 10D, (ir)

Tafel, J., *Ber.*, 1909, **42**, 3146, (synth)

Wibaut, J.P. *et al.*, *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1939, **58**, 329, (synth)

Lindeman, L.P. *et al.*, *Anal. Chem.*, 1971, **43**, 1245, (cmr)

Howe, I., *Org. Mass Spectrom.*, 1975, **10**, 767, (ms)

Brunel, J.J. *et al.*, *Tet. Lett.*, 1977, 3955, (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, MKL250

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