



>>Entry Name: 2-Methylheptane, 9CI

Synonym(s): Isooctane‡

CAS Registry Number: 592-27-8

Extra CAS Registry Numbers(s): 26635-64-3

$(\text{H}_3\text{C})_2\text{CH}(\text{CH}_2)_4\text{CH}_3$

Molecular Formula: C_8H_{18}

Molecular Weight: 114.23

Accurate Mass: 114.14085

Percentage Composition: C 84.12%; H 15.88%

Source/Synthesis: Occurs in petroleum

Melting Point: Fp -111.3°

Boiling Point: Bp 99.3°

Hazard & Toxicity: Highly flammable, fl. p. 4° , autoignition temp. 420°

Aldrich: M4794-9

Fluka: 67120

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 12A, (*nmr*)

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

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 11B, (*ir*)

Buck, F.R. *et al.*, *J. Inst. Pet.*, 1949, **35**, 631, (*synth*)

Dvoretzky, I. *et al.*, *Anal. Chem.*, 1963, **35**, 545, (*synth*)

Gallant, R.W., *Hydrocarbon Process.*, 1967, **46**, 135, (*rev, props*)

Mann, G., *Tetrahedron*, 1967, **23**, 3375, (*conformn, props*)

Beierbeck, H. *et al.*, *Can. J. Chem.*, 1977, **55**, 771, (*cmr*)