



>>Entry Name: 2,2,4-Trimethylpentane, 9CI, 8CI

Synonym(s): Isooctane‡

CAS Registry Number: 540-84-1

Extra CAS Registry Numbers(s): 26635-64-3 29222-48-8

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

Molecular Formula: C_8H_{18}

Molecular Weight: 114.23

Accurate Mass: 114.14085

Percentage Composition: C 84.12%; H 15.88%

Use/Importance: Antiknock standard for petroleum, solv. for spectroscopy etc.

Physical Description: Liq.

Melting Point: Mp -107.5°

Boiling Point: Bp 99.2°

Density: d_4^{20} 0.692

Refractive Index: n_D^{20} 1.3916

Other Data: The name isooctane is unsystematic and misleading

Hazard & Toxicity: High vapour conc. narcotic. Highly flammable, fl. p. -12° , autoignition temp. 415°

Aldrich: 36059-7

Fluka: 59050

Rare Chemicals Library: S55785-4

Sigma: T1166

Supelco: R80-1020

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 15C, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 11D, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 15C, (ir)

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

Kornblum, N. *et al.*, *J.A.C.S.*, 1978, **100**, 289, (synth)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, TLY500

Low, L.K. *et al.*, *Ethel Browning's Toxicity and Metabolism of Industrial Solvents*, 2nd edn., (ed. Snyder, R.), Elsevier, Volume 1, 1987, 312, (rev, tox)