



>>Entry Name: Dodecane, 9CI

CAS Registry Number: 112-40-3

Type of Compound Code(s): VA0050

$\text{H}_3\text{C}(\text{CH}_2)_{10}\text{CH}_3$

Molecular Formula: $\text{C}_{12}\text{H}_{26}$

Molecular Weight: 170.337

Accurate Mass: 170.20345

Percentage Composition: C 84.62%; H 15.38%

Source/Synthesis: Constit. of petroleum

Biological Source: Isol. from various essential oils

Use/Importance: Detergent feedstock, in admixture with other alkanes in C_{11} - C_{16} range

Melting Point: Fp -12°

Boiling Point: Bp 214.5° . Bp₁₀₀ 145°

Hazard & Toxicity: Fl. p. 74° , autoignition temp. 200°

Aldrich: 29787-9

Fluka: 44020

Rare Chemicals Library: S45416-8

Sigma: D4259

Supelco: R42-1012

References:

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 3B, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 3A, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 4A, (ir)

Krafft, F. *et al.*, *Ber.*, 1882, **15**, 1698, (synth)

Schrauth, W. *et al.*, *Ber.*, 1931, **64**, 1316, (synth)

Duric, R.A. *et al.*, *Spectrochim. Acta*, 1962, **18**, 1505, (ir)

Eastham, J.F. *et al.*, *J.A.C.S.*, 1963, **85**, 2171, (synth)

Org. Synth., 1973, **53**, 107, (synth)

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