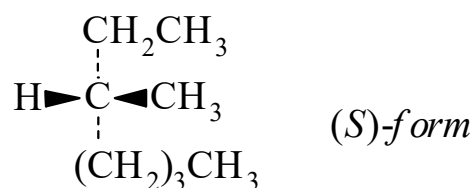




>>Entry Name: 3-Methylheptane, 9CI



CAS Registry Number: 589-81-1

Related CAS Registry Numbers(s): 111002-96-1

Molecular Formula: C₈H₁₈

Molecular Weight: 114.23

Accurate Mass: 114.14085

Percentage Composition: C 84.12%; H 15.88%

Biological Source: Constit. of *Cicer arietinum*, *Jasminum sambac* and other plant spp.

Hazard & Toxicity: Highly flammable, fl.p. -23°

Aldrich: M4795-7

Fluka: 67130

Rare Chemicals Library: S42780-2

>>Variant: (S)-form

CAS Registry Number: 6131-25-5

Molecular Formula: C₈H₁₈

Molecular Weight: 114.23

Accurate Mass: 114.14085

Percentage Composition: C 84.12%; H 15.88%

Boiling Point: Bp 118-119°

Optical Rotation: [α]_D +9.34 (neat)

>>Variant: (±)-form

Molecular Formula: C₈H₁₈

Molecular Weight: 114.23

Accurate Mass: 114.14085

Percentage Composition: C 84.12%; H 15.88%

Boiling Point: Bp 120-122°

Density: d₁₅¹⁵ 0.717

Refractive Index: n_D²⁵ 1.4022

References:

Hohenlohe-Oehringen, K., *Monatsh. Chem.*, 1962, **93**, 586, (synth)

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

Lardicci, L. *et al.*, *J.O.C.*, 1966, **31**, 1534, (synth)

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

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

Consiglio, G. *et al.*, *Tetrahedron*, 1986, **42**, 2043, (synth)