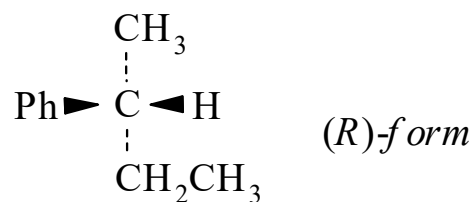




>>Entry Name: 2-Phenylbutane

Synonym(s): (1-Methylpropyl)benzene, 9CI. *sec*-Butylbenzene, 8CI



CAS Registry Number: 135-98-8

Molecular Formula: C₁₀H₁₄

Molecular Weight: 134.221

Accurate Mass: 134.10955

Percentage Composition: C 89.49%; H 10.51%

Hazard & Toxicity: Flammable, fl. p. 52°, autoignition temp. 415°. LD₅₀ (rat, orl) 2240 mg/kg

Aldrich: B9040-8

Fluka: 19630

Sigma: B7161

Supelco: R47-1795

>>Variant: (R)-form

CAS Registry Number: 5787-29-1

Molecular Formula: C₁₀H₁₄

Molecular Weight: 134.221

Accurate Mass: 134.10955

Percentage Composition: C 89.49%; H 10.51%

Boiling Point: Bp₆₀ 70-76°. Bp₂₀ 68°

Density: d₄²⁴0.87

>>Variant: (S)-form

CAS Registry Number: 5787-28-0

Molecular Formula: C₁₀H₁₄

Molecular Weight: 134.221

Accurate Mass: 134.10955

Percentage Composition: C 89.49%; H 10.51%

Boiling Point: Bp₁₅ 63°

Optical Rotation: [α]_D²⁵+28.1 (c, 1.0 in 95% EtOH aq.)

Density: d₄²⁴0.87

>>Variant: (±)-form

CAS Registry Number: 36383-15-0

Molecular Formula: C₁₀H₁₄

Molecular Weight: 134.221

Accurate Mass: 134.10955

Percentage Composition: C 89.49%; H 10.51%

Boiling Point: Bp 173-174° (170-171°). Bp₂₀ 69°

Density: d₄²¹0.86

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 3A, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 932C, (ir)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 850C, (ir)

Toussaint, N.F. *et al.*, *J.A.C.S.*, 1940, **62**, 1145, (synth)

Cram, D.J., *J.A.C.S.*, 1952, **74**, 2137, (abs config)

Adv. Chem. Ser., 1955, **15**, 27, (*props*)

Brienne, M.J. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 613, (abs config)

Friedman, H.M., *Appl. Spectrosc.*, 1970, **24**, 44, (ir)

Giardello, M.A. *et al.*, *J.A.C.S.*, 1994, **116**, 10241, (synth, pmr, cmr, S-form)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BQJ000