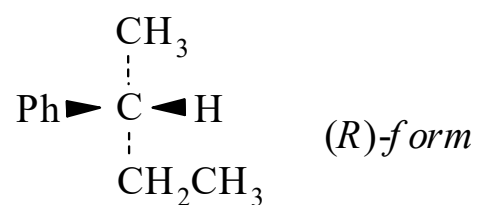




>>Entry Name: 2-Phenylbutane

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



CAS Registry Number: 135-98-8

Molecular Formula: C<sub>10</sub>H<sub>14</sub>

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°. LD<sub>50</sub> (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: C<sub>10</sub>H<sub>14</sub>

Molecular Weight: 134.221

Accurate Mass: 134.10955

Percentage Composition: C 89.49%; H 10.51%

Boiling Point: Bp<sub>60</sub> 70-76°. Bp<sub>20</sub> 68°

Density: d<sub>4</sub><sup>24</sup>0.87

>>Variant: (*S*)-form

CAS Registry Number: 5787-28-0

Molecular Formula: C<sub>10</sub>H<sub>14</sub>

Molecular Weight: 134.221

Accurate Mass: 134.10955

Percentage Composition: C 89.49%; H 10.51%

Boiling Point: Bp<sub>15</sub> 63°

Optical Rotation: [α]<sub>D</sub><sup>25</sup>+28.1 (c, 1.0 in 95% EtOH aq.)

Density: d<sub>4</sub><sup>24</sup>0.87

>>Variant: (±)-form

CAS Registry Number: 36383-15-0

Molecular Formula: C<sub>10</sub>H<sub>14</sub>

Molecular Weight: 134.221

Accurate Mass: 134.10955

Percentage Composition: C 89.49%; H 10.51%

Boiling Point: Bp 173-174° (170-171°). Bp<sub>20</sub> 69°

Density: d<sub>4</sub><sup>21</sup>0.86

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