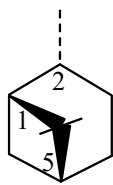




>>Entry Name: Pinane

Synonym(s): 2,7,7-Trimethylbicyclo[3.1.1]heptane



(1*R*,2*R*,5*R*)-form

CAS Registry Number: 473-55-2

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Use/Importance: Intermed. used in manuf. of terpene alcohols

Hazard & Toxicity: Autoignition temp. 273°

Fluka: 80585

>>Variant: (1*R*,2*R*,5*R*)-form

Synonym(s): (+)-*trans*-form

CAS Registry Number: 4863-59-6

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Physical Description: Oil

Optical Rotation: [α]_D +14

Fluka: 80597

>>Variant: (1*R*,2*S*,5*R*)-form

Synonym(s): (+)-*cis*-form

CAS Registry Number: 4795-86-2

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Physical Description: Oil

Boiling Point: Bp 169°

Optical Rotation: [α]_D +19

Fluka: 80593

>>Variant: (1*S*,2*R*,5*S*)-form

Synonym(s): (–)-*cis*-form

CAS Registry Number: 4755-33-3

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Physical Description: Oil

Optical Rotation: [α]_D –19.3

Fluka: 80592

>>Variant: (1*S*,2*S*,5*S*)-form

Synonym(s): (–)-*trans*-form

CAS Registry Number: 10281-53-5

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Physical Description: Oil

Optical Rotation: [α]_D –12.4

Fluka: 80595

References: