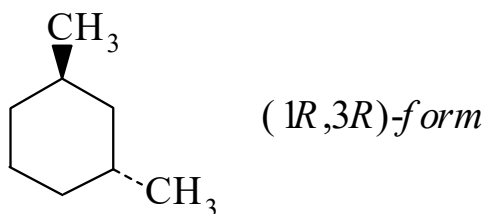




>>Entry Name: 1,3-Dimethylcyclohexane, 9CI

Synonym(s): Hexahydro-*m*-xylene



CAS Registry Number: 591-21-9

Extra CAS Registry Numbers(s): 27195-67-1

Molecular Formula: C₈H₁₆

Molecular Weight: 112.214

Accurate Mass: 112.1252

Percentage Composition: C 85.63%; H 14.37%

Aldrich: 11838-9

>>Variant: (1*R*,3*R*)-form

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

CAS Registry Number: 69685-68-3

Molecular Formula: C₈H₁₆

Molecular Weight: 112.214

Accurate Mass: 112.1252

Percentage Composition: C 85.63%; H 14.37%

Optical Rotation: $[\alpha]_{\text{D}}^{25} +70$

>>Variant: (1*RS*,3*RS*)-form

Synonym(s): (±)-*trans*-form

CAS Registry Number: 69685-67-2

Extra CAS Registry Numbers(s): 2207-03-6

Molecular Formula: C₈H₁₆

Molecular Weight: 112.214

Accurate Mass: 112.1252

Percentage Composition: C 85.63%; H 14.37%

Melting Point: Fp −90.1°

Boiling Point: Bp 124°

Refractive Index: n_{D}^{20} 1.4229

Hazard & Toxicity: Highly flammable, fl. p. 6/10°, autoignition temp. 306°

>>Variant: (1*RS*,3*SR*)-form

Synonym(s): *cis*-form

CAS Registry Number: 638-04-0

Molecular Formula: C₈H₁₆

Molecular Weight: 112.214

Accurate Mass: 112.1252

Percentage Composition: C 85.63%; H 14.37%

Melting Point: Fp −75.6°

Boiling Point: Bp 119.8-120.3°

Refractive Index: n_{D}^{25} 1.4287

Aldrich: 11836-2

References: