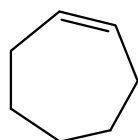




>>Entry Name: Cycloheptene

Synonym(s): Suberene‡



(Z)-form

CAS Registry Number: 628-92-2

Related CAS Registry Numbers(s): 128869-93-2

Molecular Formula: C<sub>7</sub>H<sub>12</sub>

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Hazard & Toxicity: Highly flammable, fl. p. -6°

Aldrich: 14172-0

>>Variant: (E)-form

CAS Registry Number: 45509-99-7

Molecular Formula: C<sub>7</sub>H<sub>12</sub>

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Source/Synthesis: Can be generated at low temp. and trapped

Other Data: Rapidly isom. to Z-form at r.t. UV implies substantial twist to double bond while pmr implies 180° dihedral angle of vinyl protons

>>Derivative: Diphenylisobenzofuran adduct

Melting Point: Mp 148-150°

>>Variant: (Z)-form

Molecular Formula: C<sub>7</sub>H<sub>12</sub>

Molecular Weight: 96.172

Accurate Mass: 96.0939

Percentage Composition: C 87.42%; H 12.58%

Boiling Point: Bp 115°

Density: d<sub>4</sub><sup>20</sup> 0.823

Refractive Index: n<sub>D</sub><sup>20</sup> 1.4552

>>Derivative: Diphenylisobenzofuran adduct

Melting Point: Mp 183-185°

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **1**, 58A, (nmr)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 41A, (ir)

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 59A, (ir)

Harries, C. *et al.*, *Ber.*, 1908, **41**, 1709, (synth)

Corey, E.J. *et al.*, *J.A.C.S.*, 1965, **87**, 934, (synth)

Kitching, W. *et al.*, *Tetrahedron*, 1988, **44**, 3819, (cmr)

Ermolaeva, L.I. *et al.*, *J. Mol. Struct.*, 1989, **196**, 151, (conformn)

Squillacote, M. *et al.*, *Tet. Lett.*, 1989, **30**, 6805, (E-form, uv, pmr)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, COY250