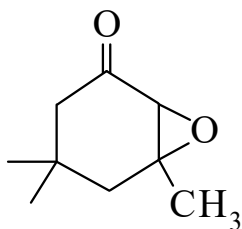




>>Entry Name: 4,4,6-Trimethyl-7-oxabicyclo[4.1.0]heptan-2-one, 9CI

Synonym(s): 2,3-Epoxy-3,5,5-trimethylcyclohexanone. Isophorone oxide



CAS Registry Number: 10276-21-8

Molecular Formula: C₉H₁₄O₂

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Aldrich: 40467-5

Rare Chemicals Library: S31125-1

>>Variant: (±)-form

Molecular Formula: C₉H₁₄O₂

Molecular Weight: 154.208

Accurate Mass: 154.09938

Percentage Composition: C 70.10%; H 9.15%; O 20.75%

Physical Description: Liq.

Boiling Point: Bp₅ 70-73°

>>Derivative: Semicarbazone

Physical Description: Cryst. (EtOH)

Melting Point: Mp 213°

References:

Org. Synth., Coll. Vol., 4, 1963, 552-553, (*synth*)

Patel, K.M. *et al.*, *Synth. Commun.*, 1975, **5**, 27-32, (*synth*)

MacAlpine, G.A. *et al.*, *Can. J. Chem.*, 1978, **56**, 308-315, (*synth*)

Tamura, Y. *et al.*, *Tet. Lett.*, 1979, 1129-1132, (*synth*)

Elings, J.A. *et al.*, *Eur. J. Org. Chem.*, 2000, 1905-1911, (*synth, pmr, cmr, ms*)