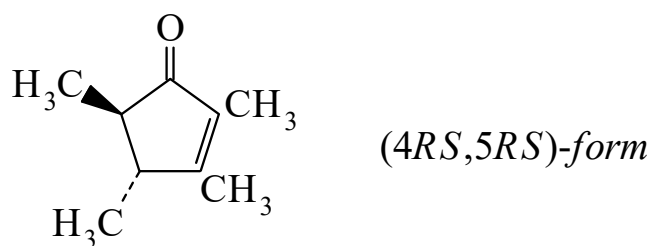




>>Entry Name: 2,3,4,5-Tetramethyl-2-cyclopenten-1-one, 9CI



CAS Registry Number: 54458-61-6

Related CAS Registry Numbers(s): 129239-77-6 129239-78-7

Molecular Formula: C₉H₁₄O

Molecular Weight: 138.209

Accurate Mass: 138.104465

Percentage Composition: C 78.21%; H 10.21%; O 11.58%

Aldrich: 27465-8

Fluka: 87795

>>Variant: (4*RS*,5*RS*)-form

Synonym(s): (±)-*trans*-form

CAS Registry Number: 34103-90-7

Molecular Formula: C₉H₁₄O

Molecular Weight: 138.209

Accurate Mass: 138.104465

Percentage Composition: C 78.21%; H 10.21%; O 11.58%

Physical Description: Pale yellow liq.

Boiling Point: Bp₁₃ 80°

Other Data: λ_{max} 242 nm (MeOH)

>>Variant: (4*RS*,5*SR*)-form

Synonym(s): (±)-*cis*-form

CAS Registry Number: 111690-89-2

Molecular Formula: C₉H₁₄O

Molecular Weight: 138.209

Accurate Mass: 138.104465

Percentage Composition: C 78.21%; H 10.21%; O 11.58%

Physical Description: Liq.

Other Data: λ_{max} 240 nm (MeOH). Not obt. pure. Has higher Bp than the *trans*-form

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 688C, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 534B, (*ir*)

DeVries, L., *J.O.C.*, 1960, **25**, 1838, (*synth, uv, ir*)

Campbell, P.H. *et al.*, *J.A.C.S.*, 1969, **91**, 6404, (*synth, ir, pmr*)

Kohl, F.X. *et al.*, *J. Organomet. Chem.*, 1984, **243**, 119, (*synth*)

Fendrick, C.M. *et al.*, *Organometallics*, 1988, **7**, 1828, (*synth, pmr*)

Yuki, T. *et al.*, *J.O.C.*, 1993, **58**, 4497, (*synth, pmr, cmr, ir*)