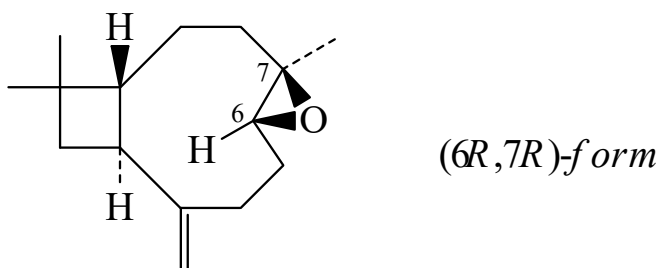




>>Entry Name: 6,7-Epoxy-3(15)-caryophyllene

ENTRY UNDER REVIEW

Synonym(s): Epoxycaryophyllene. Caryophyllene oxide. Epoxydihydrocaryophyllene



CAS Registry Number: 17627-43-9

Related CAS Registry Numbers(s): 13877-94-6

Molecular Formula: C₁₅H₂₄O

Molecular Weight: 220.354

Accurate Mass: 220.182715

Percentage Composition: C 81.76%; H 10.98%; O 7.26%

Use/Importance: Used in perfumery

>>Variant: (6R,7R)-form

Synonym(s): Caryophyllene α-oxide

CAS Registry Number: 1139-30-6

Type of Compound Code(s): W15000 VS1730

Molecular Formula: C₁₅H₂₄O

Molecular Weight: 220.354

Accurate Mass: 220.182715

Percentage Composition: C 81.76%; H 10.98%; O 7.26%

Biological Source: Constit. of oil of cloves (*Eugenia caryophyllata*). Also in oils of *Betula alba*, *Mentha piperita* and others. Major prod. of oxidn. of KGV69-V

Physical Description: Cryst.

Melting Point: Mp 63.5-64°

Optical Rotation: $[\alpha]_D^{20} -79.4$ (c, 2.32 in CHCl₃)

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) >5000 mg/kg

Aldrich: W50964-7

Fluka: 22076

Sigma: C5420

>>Variant: (6S,7S)-form

Synonym(s): Caryophyllene β-oxide

Type of Compound Code(s): VS1730

Molecular Formula: C₁₅H₂₄O

Molecular Weight: 220.354

Accurate Mass: 220.182715

Percentage Composition: C 81.76%; H 10.98%; O 7.26%

Biological Source: Minor prod. of epoxidn. KGV69-V

Melting Point: Mp 29-31 approx.°

Optical Rotation: $[\alpha]_D$ 0 (c, 2.46 in CHCl₃)

Other Data: Warnhoff appears to show the wrong configs.

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 237C, (ir)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 380A, (nmr)

Treibs, W., *Chem. Ber.*, 1947, **80**, 56, (synth)

Karrer, W. *et al.*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1930, (occur)

Warnhoff, E.W. *et al.*, *Can. J. Chem.*, 1973, **51**, 3955, (synth, pmr)

Gatilov, Yu.A. *et al.*, *Khim. Prir. Soedin.*, 1982, **18**, 715; *Chem. Nat. Compd. (Engl. Transl.)*, 677, (cryst struct, bibl)

Nishiya, K. *et al.*, *Phytochemistry*, 1992, **31**, 3511, (isol, pmr, cmr)

Heymann, H. *et al.*, *Chem. Pharm. Bull.*, 1994, **42**, 138, (isol, pmr, cmr)

Thebtaranonth, C. *et al.*, *Phytochemistry*, 1995, **40**, 125, (isol, pmr, cmr)

Sakar, M.K. *et al.*, *Fitoterapia*, 1999, **70**, 103-105, (pmr, cmr)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, CCN100