



Formula: C₁₅H₂₄

MW: 204.36

CAS: 87-44-5

MDL: MFCD00075925

TNP: TNP00558

(1R,9S)-8-METHYLEN-4,11,11-TRIMETHYL-BICYCLO[7.2.0]UNDEC-4-ENE;
8-METHYLENE-4,11,11-TRIMETHYLBICYCLO[7.2.0]UNDEC-4-ENE; B-CARYOPHYLLENE;
BETA-CARYOPHYLLEN; BETA-CARYOPHYLLENE; CARYOPHYLLENE, (-)-TRANS-;
CARYOPHYLLENE NATURAL; CARYOPHYLLENE



LogP: 6.83

LogS: -5.12

Acceptors: 0

Donors: 0

Rotation Bonds: 0

Chiral Centers: 2

N+O: 0

LIPINSKY: 3

Oil: OIL

Info: Use in perfumery

IUPAC: (1S,9R)-6,10,10-trimethyl-2-methylenebicyclo[7.2.0]undec-5-ene

Smiles: C1(C[C@H]2[C@H]1(CCC(C)=CCCC2=C))(C)C

Specification: Sesqui-Terpenoids; Biochemistry; Terpenes; Terpenes (Others)

BETA-CARYOPHYLLENE Chemical Properties:

bp 262-264 C(lit.) density 0.902 g/mL at 20 C(lit.) FEMA 2252 refractive index n₂₀/D 1.5(lit.) Fp 205 F Merck 1875 CAS DataBase Reference 87-44-5 (CAS DataBase Reference) Safety Information Risk Statements 36/37/38 Safety Statements 26-36 WGK Germany 1 RTECS DT8400000 BETA-CARYOPHYLLENE Usage And Synthesis General Description Pale yellow oily liquid with an odor midway between odor of cloves and turpentine. Air & Water Reactions Insoluble in water. Reactivity Profile The unsaturated aliphatic hydrocarbons, such as BETA-CARYOPHYLLENE, are generally much more reactive than the alkanes. Strong oxidizers may react vigorously with them. Reducing agents can react exothermically to release gaseous hydrogen. In the presence of various catalysts (such as acids) or initiators, compounds in this class can undergo very exothermic addition polymerization reactions. Fire Hazard BETA-CARYOPHYLLENE is combustible. BETA-CARYOPHYLLENE Raw materials CLOVE STEM OIL --> Cassia Aurantium P.E Catechins 8% HPLC --> EUGENIA CARYOPHYLLUS (CLOVE) LEAF OIL

Merck 13 Reference: Monograph Number: 0001890

Title: Caryophyllene

CAS Registry Number: 87-44-5

CAS Name: (1R,4E,9S)-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene

Additional Names: b-caryophyllene; trans-caryophyllene

Molecular Formula: C₁₅H₂₄

Molecular Weight: 204.35.

Percent Composition: C 88.16%, H 11.84%

Literature References: Sesquiterpenoid occurring in many essential oils and especially in clove oil, the oils from stems and flowers of *Syzygium aromaticum* (L.) Merrill & Perry (*Jambrosa caryophyllus* Niedenzu; *Eugenia caryophyllata* Thunb.), Myrtaceae. Occurs in nature as a mixture with isocaryophyllene and a-caryophyllene (humulene, q.v.). Isolation of mixture: Schreiner, Kremers, Pharm. Arch. 2, 273, 293 (1899). Existence of isomers: Deussen, Ann. 356, 1 (1907). Structure: Aebi et al., J. Chem. Soc. 1953, 3124; Ramage, Whitehead, ibid. 1954, 4336. Abs config: Barton, Nickon, ibid. 4665. Total synthesis of racemic trans/cis-forms: Corey et al., J. Am. Chem. Soc. 86, 485 (1964). Rearrangement to isocaryophyllene: Rachlin, DE 2044018 (1971 to I.F.F.), C.A. 75, 49364j (1971). Reviews: Simonsen, The Terpenes vol. III (University Press, Cambridge, 1952) pp 39-71; Barton, de Mayo, Q. Rev. Chem. Soc. 11, 197 (1957); Halsall, ibid. 16, 101 (1962).

Properties: Liquid. Has a terpene odor about midway between odor of cloves and turpentine. bp₁₄ 129-130; bp_{9.7} 118-119. [α]_{D15} -5.2. n_{D17} 1.5009; n_{D15} 1.5030. d₄₁₇ 0.9052.

Boiling point: bp₁₄ 129-130; bp_{9.7} 118-119

Optical Rotation: [α]_{D15} -5.2

Index of refraction: n_{D17} 1.5009; n_{D15} 1.5030

Density: d₄₁₇ 0.9052

Derivative Type: Dihydrochloride

Molecular Formula: C₁₅H₂₄.2HCl

Molecular Weight: 277.27.

Percent Composition: C 64.98%, H 9.45%, Cl 25.57%

Properties: mp 69-70.

Melting point: mp 69-70

Derivative Type: Nitrosochloride

Molecular Formula: C₁₅H₂₄.ClNO

Molecular Weight: 269.81.

Percent Composition: C 66.77%, H 8.97%, Cl 13.14%, N 5.19%, O 5.93%

Properties: Crystals, dec 159. [α]_{D17} -98.07.

Optical Rotation: [α]_{D17} -98.07

Derivative Type: Isocaryophyllene

CAS Registry Number: 118-65-0

Additional Names: g-Caryophyllene; cis-caryophyllene

Properties: Liquid. bp₁₉ 130; bp_{14.5} 125-125.5. [α]_{D19} -26.17. n_{D19} 1.4966. d₁₉ 0.8995. When treated with hydrogen chloride gives b-caryophyllene dihydrochloride.

Boiling point: bp₁₉ 130; bp_{14.5} 125-125.5

Optical Rotation: $[\alpha]_{D19} -26.17$

Index of refraction: $n_{D19} 1.4966$

Density: $d_{19} 0.8995$

Derivative Type: Nitrosochloride

Molecular Formula: $C_{15}H_{24}ClNO$

Molecular Weight: 269.81.

Percent Composition: C 66.77%, H 8.97%, Cl 13.14%, N 5.19%, O 5.93%

Properties: Exists in two modifications: dec 122, $[\alpha]_{D20.5} +14.71$, and dec 146, $[\alpha]_{D18} -33.69$.

Optical Rotation: $[\alpha]_{D20.5} +14.71$; $[\alpha]_{D18} -33.69$

Use: In perfumery.