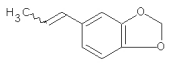

Formula: C10H10O2

MW: 162.19

CAS: 120-58-1

MDL: MFCD00005838

TNP: TNP00541

1,2-(methylenedioxy)-4-propenyl-benzen; 1,2-Methylendioxy-4-propenylbenzol; 3,4-(Methylenedioxy)-1-propenylbenzene; 3,4-(methylenedioxy)propenylbenzene; 3,4-Methylenedihydroxy-1-propenylbenzene; 3,4-methylenedioxy-1-propenylbenzene; 4-Propenyl-1,2-methylenediox

LogP: 5

LogS: -6.09

Acceptors: 2

Donors: 0

Rotation Bonds: 1

Chiral Centers: 0

N+O: 2

LIPINSKY: 4

Oil: LIQUID

Info: Isolated From Safrole. Safrole is a colorless or slightly yellow oily liquid. It is typically extracted from the root-bark or the fruit of sassafras plants in the form of sassafras oil, or synthesized from other related methylenedioxy compounds. It is the

IUPAC: isosafrole

Smiles: c12c(OCO1)ccc(/C=CC)c2

Specification: ISOSAFROLE Chemical Properties:

bp 77-86 C3.5 mm Hg(lit.) density 1.12 g/mL at 25 C(lit.) refractive index n20/D 1.573(lit.) Fp >230 F Merck 13,5244 CAS DataBase Reference120-58-1(CAS DataBase Reference) Safety Information Hazard Codes Xn Risk Statements 22-38 Safety Statements 36 WGK Germany 3 RTECS DA5950000 ISOSAFROLE Usage And Synthesis Chemical Properties:

CLEAR SLIGHTLY YELLOW LIQUID General DescriptionColorless fragrant liquid with odor of anise. Used in small quantities in root beer and sarsaparilla flavors. Reactivity ProfileISOSAFROLE may react with strong reducing agents. ISOSAFROLE Preparation ProductsPiperonyl aldehyde-->ISOEUGENOL-->BERBERINE CHLORIDE Raw materialsEtanol-->Safrole

Merck 13 Reference: Monograph Number: 0005244

Title: Isosafrole

CAS Registry Number: 120-58-1

CAS Name: 5-(1-Propenyl)-1,3-benzodioxole

Additional Names: 1,2-(methylenedioxy)-4-propenylbenzene

Molecular Formula: C10H10O2

Molecular Weight: 162.19.

Percent Composition: C 74.05%, H 6.21%, O 19.73%

Literature References: Purification and separation from safrole: Balbiano, Ber. 42, 1505 (1911); Hoering, Baum, ibid. 3082. Prepn: Bert, Compt. Rend. 213, 873 (1941); Naves, Ardizio, Bull. Soc. Chim. Fr. 1957, 1053; Fengeas, ibid. 1964, 1892; Cabiddu et al., Ann. Chim. (Rome) 52, 1261 (1962). Review and evaluation of studies of carcinogenic action in laboratory animals: IARC Monographs 10, 231-241 (1976).

Derivative Type: trans-Form

Properties: Liquid, odor of anise. bp760 253; bp100 179.5; bp20 135.6; bp3.4 85-86. mp 8.2. d420 1.1206. nD20 1.5782. uv max (96% alc): 305, 267, 259.5 nm (e 5340; 11600; 12160). Miscible with alc, ether, benzene. Sol in 8 parts of 90% alcohol.

Melting point: mp 8.2

Boiling point: bp760 253; bp100 179.5; bp20 135.6; bp3.4 85-86

Index of refraction: nD20 1.5782

Absorption maximum: uv max (96% alc): 305, 267, 259.5 nm (e 5340; 11600; 12160)

Density: d420 1.1206

Derivative Type: cis-Form

Properties: Liq. bp3.5 77-79. mp -21.5. d420 1.1182. nD20 1.5691. uv max (96% alc): 296.5, 259 nm (e 4450; 10000).

Melting point: mp -21.5

Boiling point: bp3.5 77-79

Index of refraction: nD20 1.5691

Absorption maximum: uv max (96% alc): 296.5, 259 nm (e 4450; 10000)

Density: d420 1.1182

Use: Manuf heliotropin; to modify oriental perfumes; to strengthen soap perfumes; in small quantities together with methyl salicylate in root beer and sarsaparilla flavors.