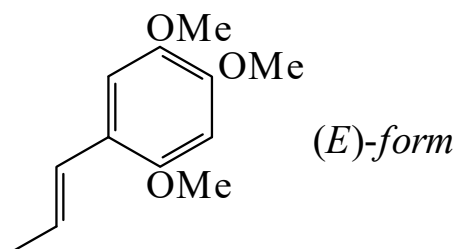




>>Entry Name: 1,2,4-Trimethoxy-5-(1-propenyl)benzene, 9CI

ENTRY UNDER REVIEW

Synonym(s): 1-(2,4,5-Trimethoxyphenyl)-1-propene. Asarone. Asarum camphor



CAS Registry Number: 494-40-6

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Biological Use/Importance: Antihypercholesterolaemic and cholelytiasic agent. Anticonvulsant, CNS depressant agent

Calculated Log P Data: Log P 2.84 (calc)

>>Variant: (E)-form

Synonym(s): α -Asarone

CAS Registry Number: 2883-98-9

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

Percentage Composition: C 69.21%; H 7.74%; O 23.05%

Biological Source: Constit. of *Asarum* spp.

Physical Description: Needles (petrol)

Melting Point: Mp 62-63°

Boiling Point: Bp 296°

UV: [neutral] $\lambda_{\max}$ 258 (log ϵ 3.82); 312 (log ϵ 4.08) (EtOH)

Hazard & Toxicity: LD₅₀ (mus, orl) 418 mg/kg. Exp. reprod. effects

Aldrich: 23128-2

Sigma: A8259

>>Derivative: 1'R*,2'R*-Epoxide

Synonym(s): 2-Methyl-3-(2,4,5-trimethoxyphenyl)oxirane. 1-(1,2-Epoxypropyl)-2,4,5-trimethoxybenzene. 1,2-Epoxy-1-(2,4,5-trimethoxyphenyl)propane. *trans*-Epoxyasarone

CAS Registry Number: 124878-08-6

Molecular Formula: C₁₂H₁₆O₄

Molecular Weight: 224.256

Accurate Mass: 224.10486

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Biological Source: Constit. of *Acorus gramineus*

Physical Description: Oil

Optical Rotation: $[\alpha]_D$ +32 (CHCl₃)

>>Derivative: 1'R*,2'S*-Epoxide

Synonym(s): *cis*-Epoxyasarone

CAS Registry Number: 321365-66-6

Molecular Formula: C₁₂H₁₆O₄

Molecular Weight: 224.256

Accurate Mass: 224.10486

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Biological Source: Constit. of *Acorus tatarinowii*

Physical Description: Oil

Optical Rotation: $[\alpha]_D^{20}$ -27.9 (c, 0.1 in CHCl₃)