



CAS Registry Number: 122-48-5

Type of Compound Code(s): WE3000 VG0010

Molecular Formula: C₁₁H₁₄O₃

Molecular Weight: 194.23

Accurate Mass: 194.094295

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Biological Source: Reputed pungent principle of ginger (*Zingiber officinale*)

Use/Importance: Flavour material used in imitation fruit flavours, ginger beer, ginger ale etc.

Physical Description: Cryst. (petrol)

Melting Point: Mp 41°

Other Data: Contrary to common assumption, free zingerone is probably not present in ginger and is certainly not its pungent principle. It is however a valuable flavouring agent

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 2580 mg/kg

Aldrich: W31240-1

>>Derivative: 3-Me ether, oxime

Molecular Formula: C₁₁H₁₅NO₃

Molecular Weight: 209.244

Accurate Mass: 209.105194

Percentage Composition: C 63.14%; H 7.23%; N 6.69%; O 22.94%

Melting Point: Mp 87.5-88.5°

>>Derivative: 3-Me ether, O-β-D-glucopyranoside

Synonym(s): Zingerone glucoside

CAS Registry Number: 64703-96-4

Type of Compound Code(s): VG0010

Molecular Formula: C₁₇H₂₄O₈

Molecular Weight: 356.372

Accurate Mass: 356.14712

Percentage Composition: C 57.30%; H 6.79%; O 35.92%

Biological Source: Isol. from Riesling vine leaf

>>Derivative: 4-Me ether

Synonym(s): 4-(3-Hydroxy-4-methoxyphenyl)-2-butanone. Isozingerone

CAS Registry Number: 77334-12-4

Type of Compound Code(s): VG0010

Molecular Formula: C₁₁H₁₄O₃

Molecular Weight: 194.23

Accurate Mass: 194.094295

Percentage Composition: C 68.02%; H 7.26%; O 24.71%

Melting Point: Mp 41-42°

Boiling Point: Bp₄ 159-160°

>>Derivative: 4-Me ether, oxime

Molecular Formula: C₁₁H₁₅NO₃

Molecular Weight: 209.244

Accurate Mass: 209.105194

Percentage Composition: C 63.14%; H 7.23%; N 6.69%; O 22.94%

Melting Point: Mp 121.5-122.5°

>>Derivative: Di-Me ether

Synonym(s): 4-(3,4-Dimethoxyphenyl)-2-butanone

CAS Registry Number: 6302-60-9

Molecular Formula: C₁₂H₁₆O₃

Molecular Weight: 208.257

Accurate Mass: 208.109945

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

Physical Description: Cryst. (EtOH or petrol)

Melting Point: Mp 55° (50°)

Boiling Point: Bp₇ 174°