



>>Entry Name: 4-Phenyl-3-buten-2-one, 9CI

ENTRY UNDER REVIEW

Synonym(s): Benzylideneacetone. Methyl styryl ketone. Benzalacetone. FEMA 2881

CAS Registry Number: 122-57-6

Related CAS Registry Numbers(s): 2887-98-1 21613-45-6 61210-87-5

PhCH=CHCOCH_3

Molecular Formula: $\text{C}_{10}\text{H}_{10}\text{O}$

Molecular Weight: 146.188

Accurate Mass: 146.073165

Percentage Composition: C 82.16%; H 6.89%; O 10.94%

Biological Source: Constit. of *Amomum globosum*, *Comptonia peregrina* and *Scutellaria baicalensis*. Present in hydrolysed soy protein

Use/Importance: Flavouring ingredient

Hazard & Toxicity: Fl. p. 66°. Mild skin irritant. LD₅₀ (rat, orl) 2031 mg/kg

Aldrich: W28810-1

Fluka: 11960

Rare Chemicals Library: S65205-9

>>Variant: (E)-form

CAS Registry Number: 1896-62-4

Molecular Formula: $\text{C}_{10}\text{H}_{10}\text{O}$

Molecular Weight: 146.188

Accurate Mass: 146.073165

Percentage Composition: C 82.16%; H 6.89%; O 10.94%

Biological Source: Isol. from the marine sponge *Plakortis halichondrioides*

Physical Description: Lustrous plates

Melting Point: Mp 42°

Boiling Point: Bp 260-262°. Bp₉ 126-128°

Aldrich: 14788-5

>>Derivative: Oxime

Extra CAS Registry Numbers(s): 21613-44-5

Molecular Formula: $\text{C}_{10}\text{H}_{11}\text{NO}$

Molecular Weight: 161.203

Accurate Mass: 161.084064

Percentage Composition: C 74.51%; H 6.88%; N 8.69%; O 9.93%

Physical Description: Needles

Melting Point: Mp 116°

>>Derivative: Phenylhydrazone

Physical Description: Yellow needles

Melting Point: Mp 156-157°

>>Derivative: Semicarbazone

Melting Point: Mp 187°

>>Variant: (Z)-form

CAS Registry Number: 937-53-1

Molecular Formula: $\text{C}_{10}\text{H}_{10}\text{O}$

Molecular Weight: 146.188

Accurate Mass: 146.073165

Percentage Composition: C 82.16%; H 6.89%; O 10.94%

Physical Description: Liq.

Melting Point: Mp -21.5°

Boiling Point: Bp_{0.2} 67-68°